Nucleons in Nuclei: Interactions, Geometry, Symmetries

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Part I

Nuclear Pairing: Exact Symmetries, Exact Solutions, Pairing as a Stochastic Process

Mathematics of the Effective Hamiltonian

The Global Structure of the N-Body Effective Hamiltonians

- The unknown ‘true’ Hamiltonian is replaced by two effective ones

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• In low-energy sub-atomic physics the theory calculations <u>without</u> considering the residual pairing are considered <u>not realistic</u>

Pairing: $\leftrightarrow \quad v^{\text{pairing}}_{\alpha\beta;\gamma\delta} \leftarrow$ **to be defined**

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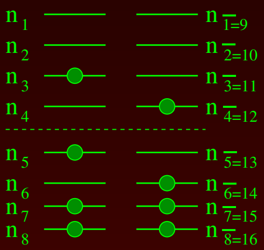
- Moreover, under the condition:

$$\textstyle\sum_j n_j = p, \quad \text{for} \quad n_j = 0 \text{ or } 1$$

each state can be seen as an integer corresponding to its binary representation

$$E = \sum_{k=1}^{n} b_k 2^{k-1} \;\rightarrow\; |0010101100010111\rangle$$



N-Body Hamiltonians and U_n-Group Generators

- N-Body Hamiltonians are functions of U_n-group generators

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- Two-body interactions lead to quadratic forms of $\hat{\mathrm{N}}_{\alpha\beta} = c^+_\alpha c_\beta$, three-body interactions to the cubic forms of $\hat{\mathrm{N}}_{\alpha\beta}$, etc.
- Hamiltonians of the N-body systems can be diagonalised within bases of the irreducible representations of unitary groups
- Solutions can be constructed that transform as the U_n-group representations thus establishing a link $\mathrm{H} \leftrightarrow U_n$-formalism

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Part II

Physics of Nuclear Pairing and Nuclear Superfluidity

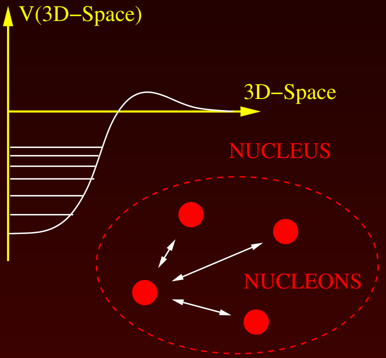
First Steps: Pairing on Top of the Mean Field

- **The first step: to solve the nuclear (HF) mean-field problem**

- **Nucleons move in a deformed one-body potential representing an everage interaction among them**

- **The one-body potentials are either parametrised or calculated using Hartree-Fock method and the single nucleon levels obtained**

$$\{e_\alpha : \alpha = 1, \ldots, n\}$$



Time-Independent Hamiltonians: Kramers Degeneracy

- **We explicitly introduce the time-reversal degeneracy**

$$\hat{T}\,\hat{H}\,\hat{T}^{-1}=\hat{H} \quad \rightarrow \quad e_\alpha = e_{\bar{\alpha}} \quad \leftrightarrow \quad |\bar{\alpha}\rangle \equiv \hat{T}\,|\bar{\alpha}\rangle$$

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- ‘Time-up’ states denoted by

$$\boxed{\{|\alpha\rangle\}}$$

- Time-reversed states by

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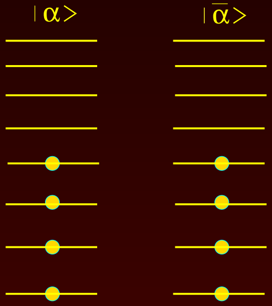
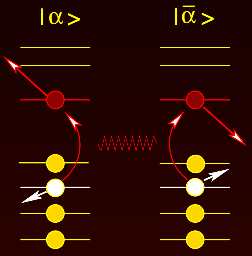


Pairing Hamiltonian: Its Experimental Background

- All the experiments show that, with no exception, all the even-even nuclei *have spin zero* in their ground states

- This implies the existence of the *universal short range interaction* that couples the time-reversed orbitals



Pairing Scheme

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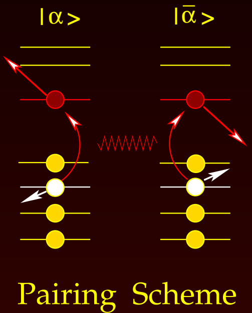


- Implied Many-Body Hamiltonian

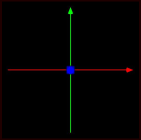
$$\hat{H} = \sum_{\alpha} e_{\alpha} \, (c^{+}_{\alpha} c_{\alpha} + c^{+}_{\bar{\alpha}} c_{\bar{\alpha}}) + \overbrace{\frac{1}{2} \sum_{\alpha\beta} \underbrace{v_{\alpha\bar{\alpha};\beta\bar{\beta}}}_{\equiv G_{\alpha\beta}} \, c^{+}_{\alpha} c^{+}_{\bar{\alpha}} \, c_{\bar{\beta}} \, c_{\beta}}^{\text{Generalized Pairing}}$$

$$|\bar{\alpha}\rangle \equiv \hat{T}|\alpha\rangle$$

Realistic Nucleonic Orbitals in the Mean-Field: A Few Examples of the Spatial Structure

Spatial Structure of Orbitals (Spherical ^{132}Sn) ($|\psi(\vec{r}\,)|^2$)

Limit 80%



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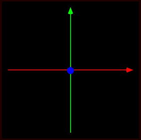

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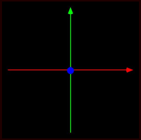

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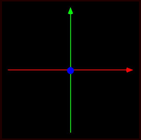

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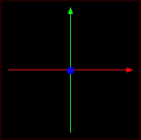

Density distribution $|\psi_\pi(\vec{r}\,)|^2 \geq$ Limit, for $\pi = [2,0,2]1/2$ orbital

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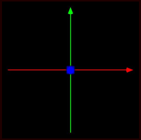

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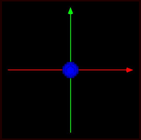

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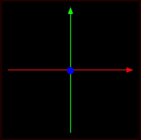

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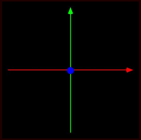

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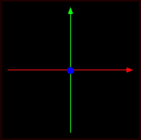

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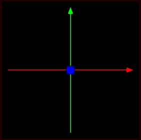

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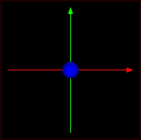

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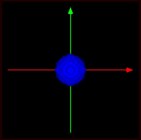

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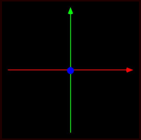

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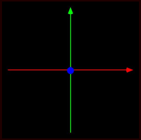

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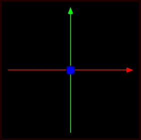

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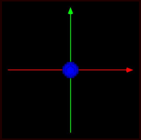

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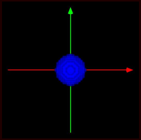

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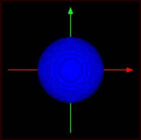

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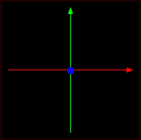

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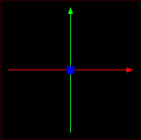

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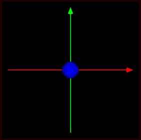

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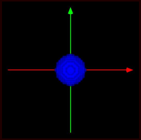

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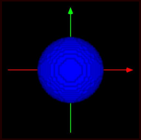

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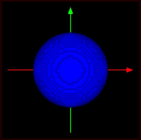

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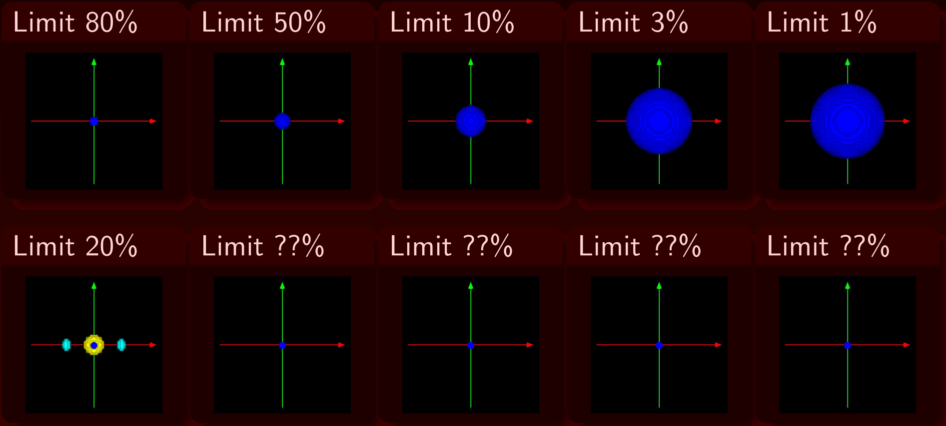

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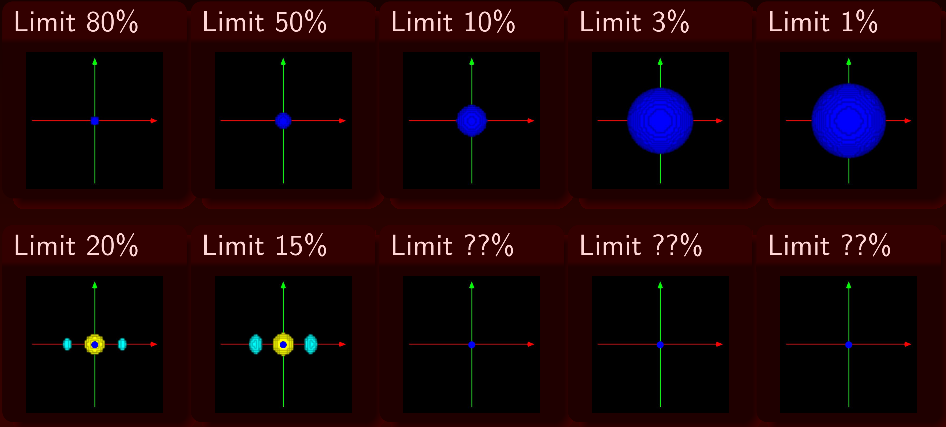

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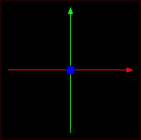

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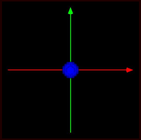

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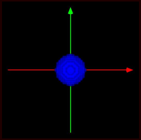

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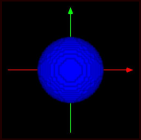

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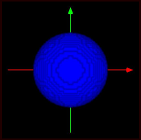

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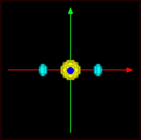

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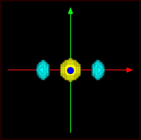

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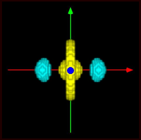

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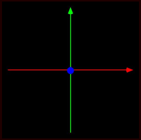

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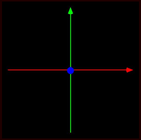

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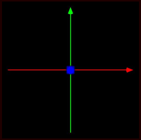

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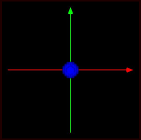

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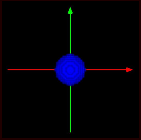

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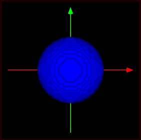

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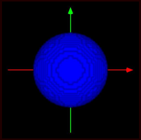

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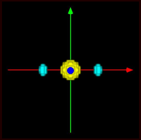

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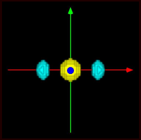

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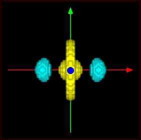

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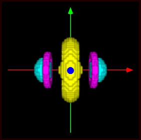
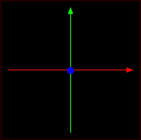
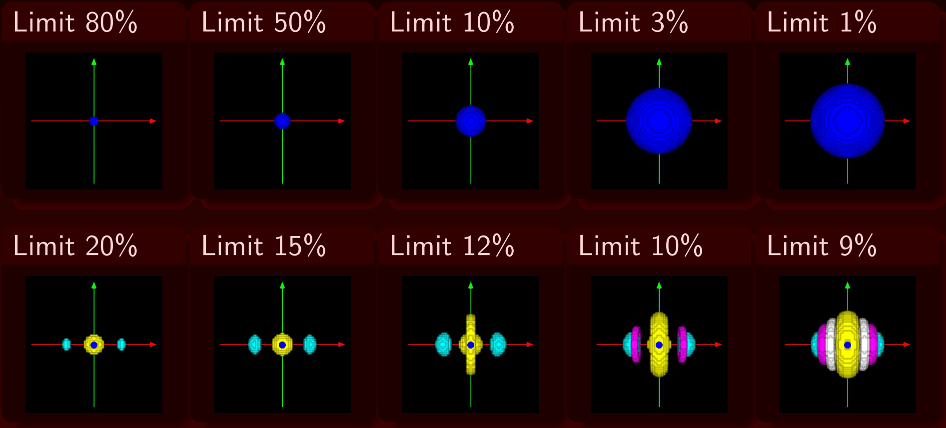


Limit ??%



Bottom: N=3 shell b-[303]7/2, w-[312]5/2, y-[321]3/2, p-[310]1/2

Spatial Structure of Orbitals (Spherical ^{132}Sn) $(|\psi(\vec{r})|^2)$



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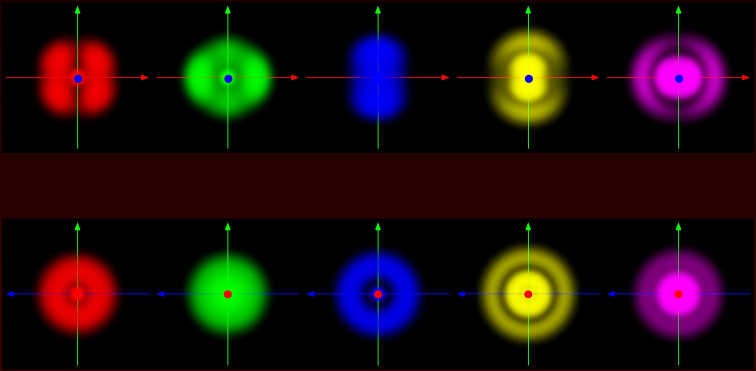
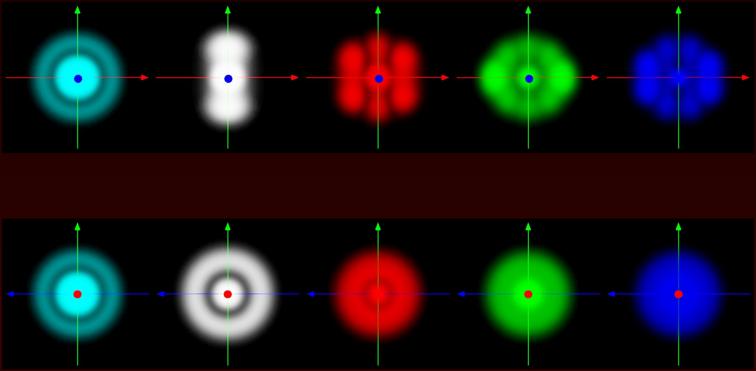
Spatial Structure of N=3 Spherical Shell ($|\psi_\nu(\vec{r})|^2$)



^{132}Sn: Distributions $|\psi_\nu(\vec{r})|^2$ for single proton orbitals. Top $\mathcal{O}_{xz}$, bottom $\mathcal{O}_{yz}$. Proton $e_\nu \leftrightarrow [\nu{=}30, 32, \ldots 38]$ for spherical shell

Spatial Structure of N=3 Spherical Shell ($|\psi_\nu(\vec{r})|^2$)



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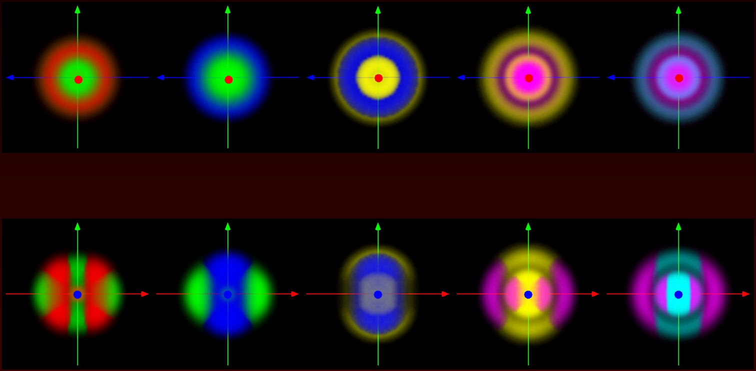
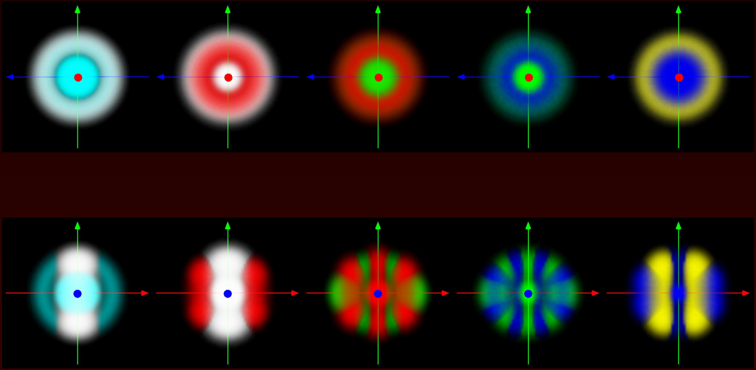


^{132}Sn: distributions $|\psi_\nu(\vec{r})|^2$ for consecutive pairs of orbitals. Top $\mathcal{O}_{xz}$, bottom $\mathcal{O}_{yz}$. Proton $e_\nu \leftrightarrow$ [n=30:32, ... 38:40], spherical shell

Spatial Structure of N=3 Spherical Shell ($|\psi_\nu(\vec{r})|^2$)



^{132}Sn: distributions $|\psi_\nu(\vec{r})|^2$ for consecutive pairs of orbitals. Top $\mathcal{O}_{xz}$, bottom $\mathcal{O}_{yz}$. Proton $e_\nu \leftrightarrow [n=40:42, \ldots\ 48:50]$, spherical shell

Dichotomic Symmetries of Pairing

Natural Dichotomic Symmetries: Time Reversal...

- There exist one-body dichotomic symmetries $\hat{S}_1 \equiv \hat{T}, \hat{R}_x, \hat{S}_x, \ldots$ where the subscript "1" refers to the one-body interaction

$$\hat{\mathbf{H}}_1 = \sum_{\alpha\beta} \langle\alpha|\hat{\mathbf{h}}_1|\beta\rangle \; \mathbf{c}_\alpha^+ \mathbf{c}_\beta \quad \text{and} \quad [\hat{\mathbf{S}}_1, \hat{\mathbf{h}}_1] = \mathbf{0}$$

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$$\boxed{\hat{S}_1^2 = -1 \rightarrow s_\alpha = \pm i}$$

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$$\boxed{\hat{\mathbf{h}}_1|\alpha, \mathbf{s}_\alpha\rangle = \mathbf{e}_{\alpha,\ \mathbf{s}_\alpha}|\alpha, \mathbf{s}_\alpha\rangle, \quad \leftrightarrow \quad \hat{\mathbf{S}}_1|\alpha, \mathbf{s}_\alpha\rangle = \mathbf{s}_\alpha|\alpha, \mathbf{s}_\alpha\rangle}$$

Exploiting the Natural Dichotomic Symmetries

- Therefore, there are 16 types of the two-body matrix elements, distinguished by the eigenvalues $s_\alpha = \pm i$

$$\hat{H} = \sum_\alpha \varepsilon_\alpha (c^+_{\alpha+} c_{\alpha+} + c^+_{\alpha-} c_{\alpha-}) + \tfrac{1}{2} \sum_{\alpha\beta} \sum_{\gamma\delta} \underbrace{\langle \alpha\pm, \beta\pm | \hat{h}_2 | \gamma\pm, \delta\pm \rangle}_{\text{16 families}} c^+_{\alpha\pm} c^+_{\beta\pm} c_{\delta\pm} c_{\gamma\pm}$$

- Since the residual two-body interactions are often assumed scalar, it follows that for the two-body operator $\hat{S}_2$, the analogue of $\hat{S}_1$

$$\boxed{\hat{S}_2 \equiv \hat{S}_1 \otimes \hat{S}_1 \quad \to \quad [\hat{h}_2, \hat{S}_2] = 0}$$

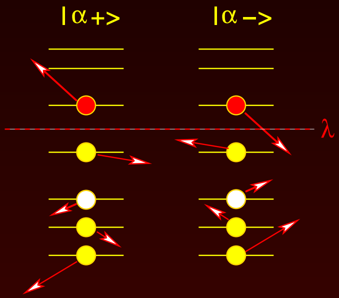
- This implies that half of the matrix elements above simply vanish

$$\langle \alpha\pm, \beta\pm | \hat{h}_2 | \gamma\pm, \delta\pm \rangle \sim \delta_{s_\alpha \cdot s_\beta,\; s_\gamma \cdot s_\delta}$$

Exploiting Dichotomic Symmetries and Pairing

- Furthermore, because of the specific form of the nuclear pairing Hamiltonian half of the above 8 types of matrix elements are absent

$$\langle \alpha+, \beta+ | \hat{h}_2 | \gamma-, \delta- \rangle = 0$$
$$\langle \alpha-, \beta- | \hat{h}_2 | \gamma+, \delta+ \rangle = 0$$
$$\langle \alpha+, \beta+ | \hat{h}_2 | \gamma+, \delta+ \rangle = 0$$
$$\langle \alpha-, \beta- | \hat{h}_2 | \gamma-, \delta- \rangle = 0$$



Exploiting Dichotomic Symmetries and Pairing

- Examples of the vanishing matrix elements

$$\langle \alpha+, \beta+ | \hat{h}_2 | \gamma-, \delta- \rangle = 0$$

$$\langle \alpha-, \beta- | \hat{h}_2 | \gamma+, \delta+ \rangle = 0$$

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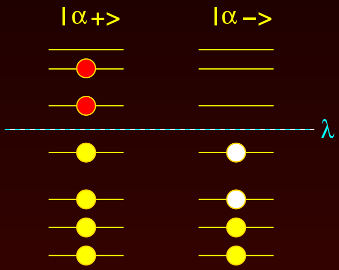

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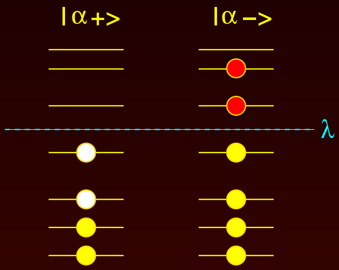

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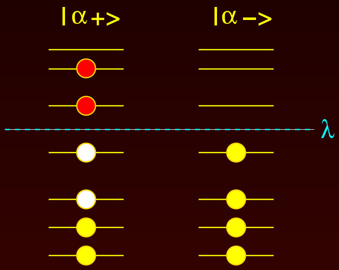

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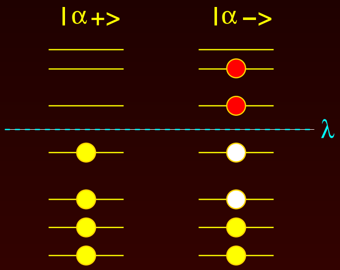


Final Structure of the Nuclear Pairing Hamiltonian

- Then the non-vanishing terms can be divided into four families

$$\begin{aligned}\hat{H}_2 \quad = \quad & \tfrac{1}{2}\sum_{\alpha+\beta-}\sum_{\gamma-\delta+} \langle\alpha+,\beta-|\hat{h}_2|\gamma-,\delta+\rangle\; c^+_{\alpha+} c^+_{\beta-}\; c_{\delta+} c_{\gamma-} \\ + \quad & \tfrac{1}{2}\sum_{\alpha+\beta-}\sum_{\gamma+\delta-} \langle\alpha+,\beta-|\hat{h}_2|\gamma+,\delta-\rangle\; c^+_{\alpha+} c^+_{\beta-}\; c_{\delta-} c_{\gamma+} \\ + \quad & \tfrac{1}{2}\sum_{\alpha-\beta+}\sum_{\gamma-\delta+} \langle\alpha-,\beta+|\hat{h}_2|\gamma-,\delta+\rangle\; c^+_{\alpha-} c^+_{\beta+}\; c_{\delta+} c_{\gamma-} \\ + \quad & \tfrac{1}{2}\sum_{\alpha-\beta+}\sum_{\gamma+\delta-} \langle\alpha-,\beta+|\hat{h}_2|\gamma+,\delta-\rangle\; c^\dagger_{\alpha-} c^\dagger_{\beta+}\; c_{\delta-} c_{\gamma+}\end{aligned}$$

- It turns out that the full Hamiltonian

$$\hat{H} \equiv \sum_{\alpha} e_\alpha(\hat{c}^+_\alpha \hat{c}_\alpha + \hat{c}^+_{\bar{\alpha}} \hat{c}_{\bar{\alpha}}) + \hat{H}_2$$

cannot connect the states that differ in terms of occupation of the "+" and "-" family states

We have just obtained the modern version of the Nuclear Pairing Hamiltonian

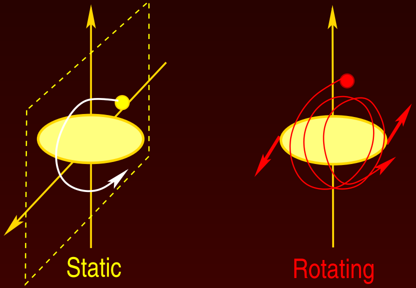
We have just obtained the modern version of the Nuclear Pairing Hamiltonian

In what sense are the paired-nuclei super-fluid?

Collective Rotation, Moments of Inertia

- The first rotational transition energies are very low; for very heavy nuclei such energies $\Delta e_R \sim 10^{-2}$ MeV. This energy is contributed by all the nucleons; a contribution *per nucleon*, is

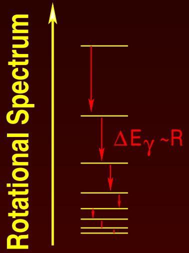
$$\delta e_R \equiv \Delta e_R / A \sim 10^{-2}\ \mathrm{MeV}/A \sim 10^{-4}\ \mathrm{MeV}$$

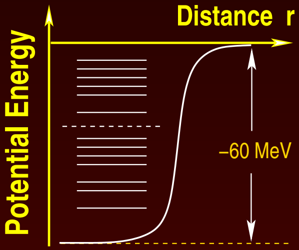


Collective Rotation, Moments of Inertia

- These energies should be compared to the average kinetic energies of nucleons in the mean-field potential of the typical depth of $V_0 \sim -60$ MeV
- A nucleon of, say, $e_\alpha \approx -25$ MeV, has the kinetic energy of the order of

$$\boxed{\langle \hat{t}\,\rangle \sim t_\alpha \sim 35\ \text{MeV}} \quad \text{so that} \quad V_0 + \langle \hat{t}\,\rangle \sim e_\nu \approx -25\ \text{MeV}$$





Collective Rotation, Moments of Inertia

- Consider explicitly a one-dimensional rotation about $\mathcal{O}_x$-axis. One may show that the perturbation is $\delta v = \hbar\omega_x \cdot \hat{j}_x$
- Consequently the second order energy contribution is

$$E_0^{(2)} = (\hbar\omega_x)^2 \sum_{mi} \frac{|(m|\hat{j}_x|i)|^2}{e_i^{(0)} - e_m^{(0)}} \quad \text{compared to} \quad E_0^{(2)} = \frac{1}{2}\mathcal{J}_x\,\omega_x^2$$

- Comparison gives

$$\boxed{\mathcal{J}_x = 2\,\hbar^2 \sum_{mi} \frac{|(m|\hat{j}_x|i)|^2}{e_i^{(0)} - e_m^{(0)}} \approx \mathcal{J}_x^{rig.} = \int_V [y^2 + z^2]\rho(\vec{r})d^3\vec{r} \neq \mathcal{J}_x^{exp.}}$$

Collective Rotation, Moments of Inertia

- Repeating the 2^{nd}-order perturbation calculation with pairing we obtain

$$\mathcal{J}_x^{pair} = 2\,\hbar^2 \sum_{\mu\nu} |\langle\mu|\hat{j}_x|\nu\rangle|^2 \frac{(u_\mu v_\nu - u_\nu v_\mu)^2}{E_\mu + E_\nu} \approx 0.5 \cdot \mathcal{J}_x^{rig.} \approx \mathcal{J}_x^{exp.}$$

- By definition, within the nuclear Bardeen-Cooper-Schrieffer approach

$$E_\mu = \sqrt{(e_\mu - \lambda)^2 + \Delta^2}, \;\; v_\mu^2 = \tfrac{1}{2}\left[1 - (e_\mu - \lambda)/E_\mu\right] \text{ and } v_\mu^2 + u_\mu^2 = 1$$

- As the pairing gap $\Delta \to \infty$ we find

$$f_{\mu\nu} \equiv \frac{(u_\mu v_\nu - u_\nu v_\mu)^2}{E_\mu + E_\nu} \overset{\Delta\to\infty}{\longrightarrow} 0 \quad \leftrightarrow \quad \boxed{\mathcal{J}_x^{pair} \to 0}$$

- *When this happens we say that system approaches the super-fluid regime*

Part III

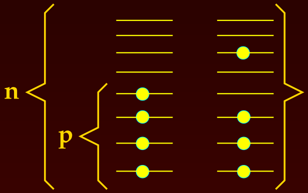
A Lesson on the Exact Solutions of the Realistic Pairing Problem

Pairing, Fock-Space and Associated Notation

- **Nuclear wave functions must be totally anti-symmetrised**
- **We formulate the problem of the motion in the Fock space**
- **We use the many-body occupation-number representation**

$$\Psi_{mb} = (c^+_{\alpha_1})^{p_{\alpha_1}} \, (c^+_{\alpha_2})^{p_{\alpha_2}} \, \ldots \, (c^+_{\alpha_n})^{p_{\alpha_n}} \, |0> \; \leftrightarrow \; |p_{\alpha_1}, \, p_{\alpha_2}, \, \ldots \, p_{\alpha_n}\rangle$$

$$p_\alpha = 0 \text{ or } 1, \quad \sum_{j=1}^{n} p_{\alpha_j} = p$$



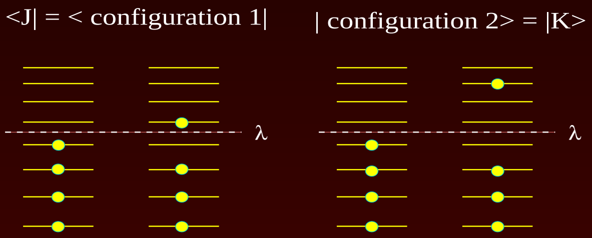
$|11 \; 11 \; 11 \; 10 \; 00 \; 01 \; 00 \; 00>$

- Computer algorithm is constructed using bit-manipulations

Particular Symmetries of the Pairing Hamiltonian

- **$\hat{H}$ does not couple states differing in particle-hole structure**
- **$\hat{H}$ does not couple states differing by 2 or more excited pairs**

$$\hat{H} = \sum_{\alpha} e_{\alpha} c^{+}_{\alpha} c_{\alpha} + \sum_{\alpha,\beta>0} G_{\alpha,\beta}\, c^{+}_{\beta}\, c^{+}_{\bar{\beta}}\, c_{\bar{\alpha}} c_{\alpha}$$



$$\boxed{\langle J|\hat{H}|K\rangle = 0}$$

Pairing Hamiltonian and the U(n)-Generators

- It follows that upon identifying $\hat{n}_{\alpha\beta} \equiv \hat{c}^+_\alpha \hat{c}_\beta \leftrightarrow \hat{g}_{\alpha\beta}$

$$\hat{H} = \sum_{\alpha>0}^{n} e'_\alpha \, (\hat{g}_{\alpha,\alpha} + \hat{g}_{\bar{\alpha},\bar{\alpha}}) - \tfrac{1}{2} \sum_{\alpha,\beta>0}^{n} G_{\alpha,\beta} \, \hat{g}_{\beta,\bar{\alpha}} \, \hat{g}_{\bar{\beta},\alpha}$$

- Introduce linear Casimir operator

$$\text{Particle No. Operator} \rightarrow \hat{N} = \textstyle\sum_\alpha^n \hat{n}_{\alpha\alpha}$$

$$\text{U(n) Casimir Operator} \rightarrow \hat{C} = \textstyle\sum_\alpha^n \hat{g}_{\alpha\alpha}$$

$$\hat{C} \equiv \sum_{\alpha}^{n} \hat{g}_{\alpha\alpha} = \sum_{\alpha+}^{N_+} \hat{g}_{\alpha+,\alpha+} + \sum_{\alpha-}^{N_-} \hat{g}_{\alpha-,\alpha-} \equiv \hat{\mathcal{N}}_1^+ + \hat{\mathcal{N}}_1^-$$

New Particle-Like Operators: $\hat{\mathcal{N}}_1^+$ and $\hat{\mathcal{N}}_1^-$

- One verifies that operators $\hat{\mathcal{N}}_1^+$ and $\hat{\mathcal{N}}_1^-$ are linearly independent

$$[\hat{H}, \hat{\mathcal{N}}_1^+] = 0, \quad [\hat{H}, \hat{\mathcal{N}}_1^-] = 0, \quad [\hat{\mathcal{N}}_1^+, \hat{\mathcal{N}}_1^-] = 0$$

- Introduce two linear combinations

$$\hat{\mathcal{N}}_1 \equiv \hat{\mathcal{N}}_1^+ + \hat{\mathcal{N}}_1^- \quad \text{and} \quad \hat{\mathcal{P}}_1 \equiv \hat{\mathcal{N}}_1^+ - \hat{\mathcal{N}}_1^-$$

- We show straightforwardly that

$$[\hat{H}, \hat{\mathcal{N}}_1] = 0, \quad [\hat{H}, \hat{\mathcal{P}}_1] = 0$$

- The Hamiltonian $\hat{H}$ is said to be $\hat{\mathcal{P}}_1$-symmetric

New Particle-Like Operators: $\hat{\mathcal{N}}_1^+$ and $\hat{\mathcal{N}}_1^-$

- Recall: Operator $\hat{\mathcal{P}}_1 \equiv \hat{\mathcal{N}}_1^+ - \hat{\mathcal{N}}_1^-$ gives the difference between the occupation of states $s_\alpha = +i$ and $s_\alpha = -i$
- It follows that the possible eigenvalues of $\mathcal{P}_1$ are

$$\mathcal{P}_1 = p,\ p-2,\ p-4,\ \dots,\ -p$$

for a system of p particles on n levels with $p \leq n/2$, and

$$\mathcal{P}_1 = (n-p),\ (n-p-2),\ (n-p-4),\ \dots,\ -(n-p)$$

for a system for which $n/2 \leq p \leq n$

- Hamiltonian matrix splits into blocks with eigenvalues $\mathcal{P}_1$; one shows that

$$\boxed{\dim(\mathcal{P}_1) = C^n_{\frac{p+\mathcal{P}_1}{2}}\, C^n_{\frac{p-\mathcal{P}_1}{2}}}$$

Illustration of the Effect of the $\mathcal{P}_1$-Symmetry

• Example of Fock-space dimensions for $p = 16$ particles on $n = 32$ levels; the dimension of the full space is $C_{16}^{32} = 601\ 080\ 390$

$\mathcal{P}_1$-value	Dimension
0	165 636 900
$\pm$ 2	130 873 600
$\pm$ 4	64 128 064
$\pm$ 6	19 079 424
$\pm$ 8	3 312 400
$\pm$ 10	313 600
$\pm$ 12	14 400
$\pm$ 14	256
$\pm$ 16	1

New Particle-Pair-Like Operators: $\hat{\mathcal{N}}_2^+$ and $\hat{\mathcal{N}}_2^-$

- Our Hamiltonian does not couple states that differ in terms of the *numbers of pairs*; the number of broken pairs (seniority) is conserved
- In analogy with the previous case we define *two-body* operators

$$\hat{\mathcal{N}}_2^+ \equiv \sum_{i=1}^{N} c_{\alpha_i}^+ c_{\bar{\alpha}_i}^+ c_{\bar{\alpha}_i} c_{\alpha_i} \quad \text{and} \quad \hat{\mathcal{N}}_2^- \equiv \sum_{i=1}^{N} (1 - c_{\alpha_i}^+ c_{\bar{\alpha}_i}^+ c_{\bar{\alpha}_i} c_{\alpha_i})$$

- Following the same analogy we also define the linear combinations

$$\hat{\mathcal{N}}_2 = \hat{\mathcal{N}}_2^+ + \hat{\mathcal{N}}_2^- \quad \text{and} \quad \hat{\mathcal{P}}_2 = \hat{\mathcal{N}}_2^+ - \hat{\mathcal{N}}_2^-$$

New Particle-Pair-Like Operators: $\hat{\mathcal{N}}_2^+$ and $\hat{\mathcal{N}}_2^-$

- One can verify straightforwardly that

$$[\hat{H},\hat{\mathcal{N}}_2^+]=0 \quad \text{and} \quad [\hat{H},\hat{\mathcal{N}}_2^-]=0 \quad \text{and} \quad [\hat{\mathcal{N}}_2^+,\hat{\mathcal{N}}_2^-]=0$$

- It then follows immediately that

$$[\hat{H},\hat{\mathcal{N}}_2]=0 \quad \text{and} \quad [\hat{H},\hat{\mathcal{P}}_2]=0 \quad \text{while} \quad [\hat{\mathcal{P}}_1,\hat{\mathcal{P}}_2]=0$$

- The Hamiltonian $\hat{H}$ is said to be $\hat{\mathcal{P}}_2$-symmetric

New Particle-Pair-Like Operators: $\hat{\mathcal{N}}_2^+$ and $\hat{\mathcal{N}}_2^-$

- By counting numbers of pairs we obtain eigen-values of $\hat{\mathcal{P}}_2$-operator
- For p particles on n levels, and $p \leq n/2$:

$$\mathcal{P}_2 = p - n,\ p - 2 - n,\ \ldots,\ -n$$

- For p particles on n levels, and $n/2 \leq p \leq n$:

$$\mathcal{P}_2 = p - n,\ p - 2 - n,\ \ldots,\ 2(p - n) - n$$

- The dimensions of a given block characterized by the quantum numbers $\mathcal{P}_1$ and $\mathcal{P}_2$ are given by:

$$\boxed{\dim(\mathcal{P}_2, \mathcal{P}_1) = C^{n}_{\frac{p-n-\mathcal{P}_2+\mathcal{P}_1}{2}}\ C^{n-\frac{p-n-\mathcal{P}_2+\mathcal{P}_1}{2}}_{\frac{p-n-\mathcal{P}_2-\mathcal{P}_1}{2}}\ C^{2n-p+\mathcal{P}_2}_{\frac{n+\mathcal{P}_2}{2}}}$$

New Particle-Pair-Like Operators: $\hat{\mathcal{N}}_2^+$ and $\hat{\mathcal{N}}_2^-$

- The Hamiltonian blocks for $p = 16$ particles on $n = 32$ levels; the dimension of the full space is $C_{16}^{32} = 601\ 080\ 390$

Seniority	$\mathcal{P}_2$	Dimension	$\mathcal{P}_1$-values	Dimension
0	0	12 870	0	12 870
2	−2	1 647 360	0	823 680
			± 2	411 840
4	−4	26 906 880	0	10 090 080
			± 2	6 726 720
			± 4	1 681 680
6	−6	129 153 024	0	40 360 320
			± 2	30 270 240
			± 4	12 108 096
			± 6	2 018 016
8	−8	230 630 400	0	63 063 000
			± 2	50 450 400
			± 4	25 225 200
			± 6	7 207 200
			± 8	900 900
...	...	...	...	...

Yet Another Symmetry: $\mathcal{P}_{12}$-Symmetry

- Define $\mu_i \equiv 2i - 2$ associated with doubly-degenerate levels ε_i
- Define the weight factors: $\alpha_i \to 2^{\mu_i}$ and $\bar{\alpha}_i \to 2^{\mu_i+1}$
- Define operators

$$\hat{\mathcal{N}}_{12}^{+} \equiv \sum_{i=1}^{n} (2^{\mu_i} c_{\alpha_i}^{+} c_{\alpha_i} + 2^{\mu_i+1} c_{\bar{\alpha}_i}^{+} c_{\bar{\alpha}_i})$$

$$\hat{\mathcal{N}}_{12}^{-} \equiv \sum_{i=1}^{n} (2^{\mu_i} + 2^{\mu_i+1}) c_{\alpha_i}^{+} c_{\bar{\alpha}_i}^{+} c_{\bar{\alpha}_i} c_{\alpha_i}$$

$$\hat{\mathcal{P}}_{12} \equiv \hat{\mathcal{N}}_{12}^{+} - \hat{\mathcal{N}}_{12}^{-}$$

Yet Another Symmetry: $\mathcal{P}_{12}$-Symmetry

- One can show that

$$[\hat{\mathcal{P}}_1, \hat{\mathcal{P}}_2] = 0 \quad \text{and} \quad [\hat{\mathcal{P}}_1, \hat{\mathcal{P}}_{12}] = 0 \quad \text{and} \quad [\hat{\mathcal{P}}_2, \hat{\mathcal{P}}_{12}] = 0$$

- ... and that for our general pairing Hamiltonian $\hat{H}$ we have

$$[\hat{H}, \hat{\mathcal{P}}_1] = 0 \quad \text{and} \quad [\hat{H}, \hat{\mathcal{P}}_2] = 0 \quad \text{and} \quad [\hat{H}, \hat{\mathcal{P}}_{12}] = 0$$

- The Hamiltonian $\hat{H}$ is said to be $\hat{\mathcal{P}}_{12}$-symmetric

How Powerful This Approach Is Shows an Example:

- The property just observed allows for significant simplifications

Example: 16 particles on 32 levels

Total dimension of H $\Rightarrow$ 601 080 390 $\times$ 601 080 390

Seniority	P_2	Total Dimension	Nb. of sub-blocs	Sub-bloc dimension
0	0	12 870	1	12 870
2	-2	1 647 360	480	3 432
4	-4	26 906 880	29 120	924
6	-6	129 153 024	512 512	252
8	-8	230 630 400	3 294 720	70
10	-10	164 003 840	8 200 192	20
12	-12	44 728 320	7 454 720	6
14	-14	3 932 160	1 966 080	2
16	-16	65 536	65 536	1

Details in: H. Molique and J. Dudek, Phys. Rev. C56, 1795 (1997)

Part IV

Cooper-Pairs as Brownian Particles

From Quantum Mechanics to Stochastic Processes

- Consider a system composed of p-particles on n nucleonic levels
- The implied Fock space contains $\mathcal{N} = C_p^n$ many-body states

$$\{|\Phi_K>;\ K = 1, 2, \dots \mathcal{N}\}$$

- The symbols represent $\mathcal{N}$ physical configurations $\{\mathcal{C}_K\}$ of the type

$$\{\mathcal{C}_K\} \leftrightarrow \{|11\,10\,00\,01\ \ \dots >_K;\ K = 1, 2, \dots \mathcal{N}\}$$

- The use of the P-symmetries allows to diagonalize exactly *and easily*, with the help of the Lanczos method, the Hamiltonian matrices

$$< \Phi_K|\,\hat{H}\,|\Phi_M > \text{ of dimensions } \mathcal{N}_b \sim 10^{\,9} \text{ to } 10^{(12\rightarrow 15)}$$

An alternative, stochastic method is free from the disc-space limitations

An alternative, stochastic method is free from the disc-space limitations

This Stochastic Method is based on fundamentally different concepts

Nuclear Pairing as a Stochastic Process

- Starting from now on we assume that the system evolves under the influence of Hamiltonian $\hat{H}$ in terms of the single-pair transitions

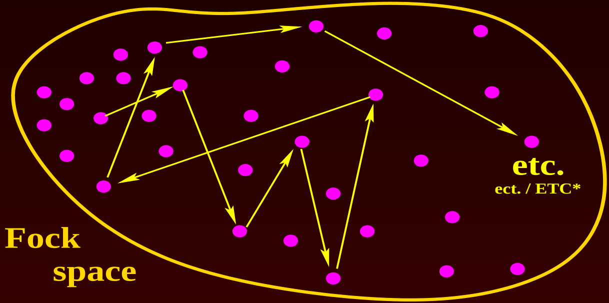
- We suggest that there exist a universal probability distribution depending on the transition energy only

$$P_{K\to K'} = P(\Delta E_{K,K'}); \quad \Delta E_{K,K'} = |E_K - E_{K'}|$$

In other words: we assume that single-pair transition probabilities are neither dependent on the particular configuration nor on the history of the process

Nuclear Pairing as a Stochastic Process

- The just formulated assumptions reduce the evolution of such a system to that of the Markov process



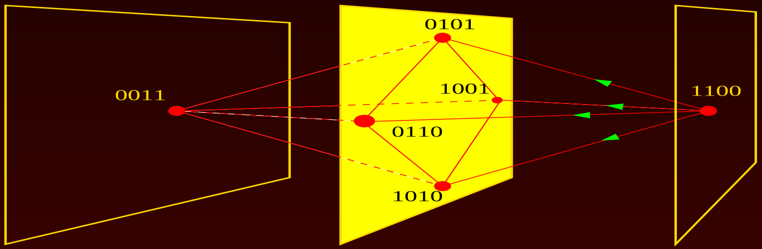
- Consequently we are going to consider the underlying physical process in terms of the random walk through the Fock space

Nuclear Pairing as a Stochastic Process

- An example of Fock space corresponding to 4 particles on 8 levels

$$\{|\Phi_K\rangle\} = \{|1100\rangle, |1010\rangle, |1001\rangle, |0110\rangle, |0101\rangle, |0011\rangle\}$$

- We have the following possible transitions:



- *To simplify the illustration we use the compact notation:*

1 $\longrightarrow$ *one* pair *present;* *0* $\longrightarrow$ *one* pair *absent*

Fock-State Occupation Probabilities

- Suppose Hamiltonian $\hat{H}$ has been diagonalised in the Fock space

$$\hat{H}\,|\Psi_K\rangle = E_K\,|\Psi_K\rangle \;\rightarrow\; |\Psi_K\rangle = \sum_{L=1}^{\mathcal{N}_b} C_{K,L}\,|\Phi_L\rangle$$

- The *quantum probability* of finding $|\Psi_K\rangle$ in one of its Fock-basis states $|\Phi_L\rangle$ is

$$\mathcal{P}_L^q = |C_{K,L}|^2 \quad (\text{for a given } |\Psi_K\rangle)$$

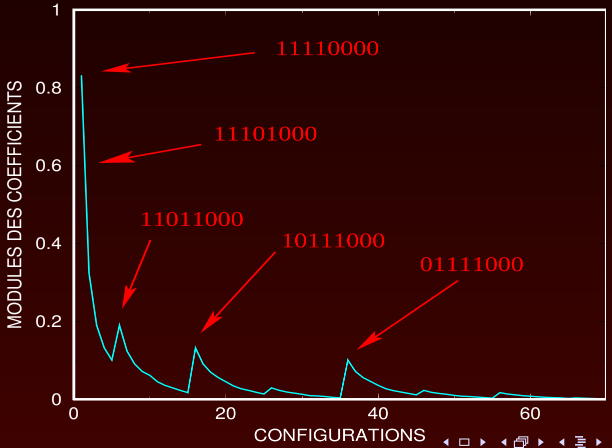
- The *stochastic probability* of finding $|\Psi_K\rangle$ in one of its Fock-basis states $|\Phi_L\rangle$ is

$$\mathcal{P}_L^s = \mathcal{N}_L/\mathcal{N}_{total} \quad (\text{for a given } |\Psi_K\rangle)$$

where $\mathcal{N}_L \longrightarrow$ the number of occurrences of $|\Phi_K\rangle$ along the random walk and $\mathcal{N}_{total}$ = the total 'length' of the random walk

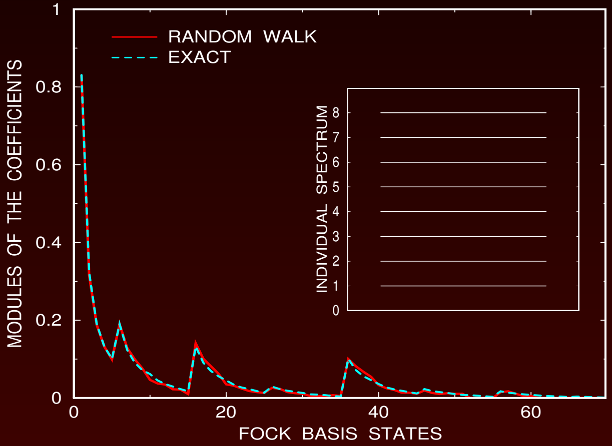
Example: Exact Quantum Occupation Probabilities

- $p = 8$ particles on $n = 16$ levels $\{\mathcal{N}_b = 70$ Fock $|\Phi_K\rangle$ states$\}$ on an equidistant model spectrum: *the ground-state wave-function*



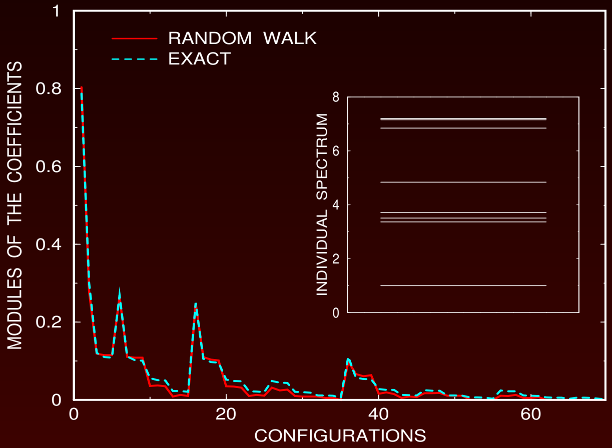
Stochastic vs. Quantum Occupation Probabilities

- 8 particles on 16 levels ($\mathcal{N}_{it}$ = 10 000 iterations)



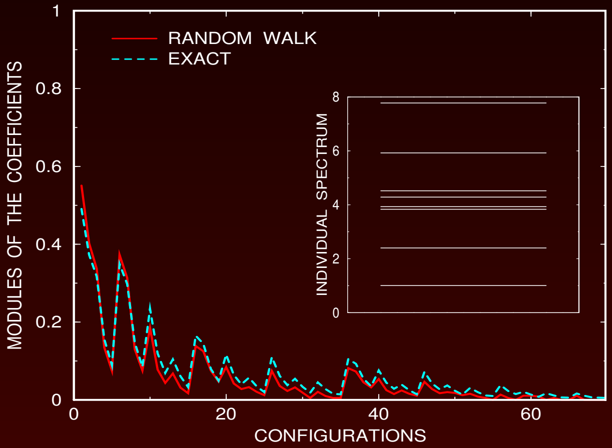
Stochastic vs. Quantum Occupation Probabilities

- 8 particles on 16 levels ($\mathcal{N}_{it}$ = 10 000 iterations) - Case 2



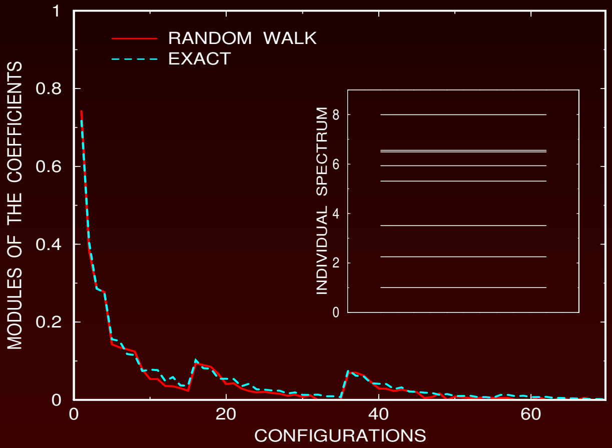
Stochastic vs. Quantum Occupation Probabilities

- 8 particles on 16 levels ($\mathcal{N}_{it} = 10\ 000$ iterations) - Case 3



Stochastic vs. Quantum Occupation Probabilities

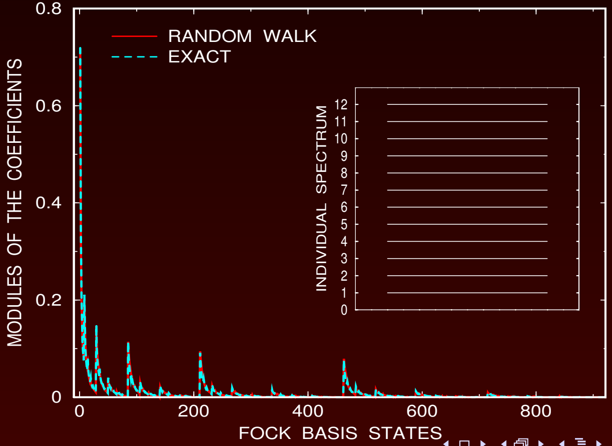
- 8 particles on 16 levels ($\mathcal{N}_{it} = 10\ 000$ iterations) - Case 4



Stochastic vs. Quantum Occupation Probabilities

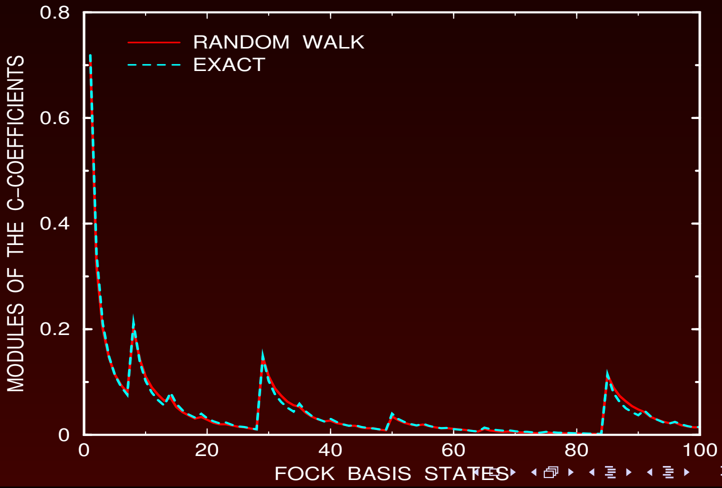
- 12 particles on 24 levels ($\mathcal{N}_{it} = 50\ 000$ iterations)

  Fock space dimension $\mathcal{N}(24/12) = 2\ 704\ 156$



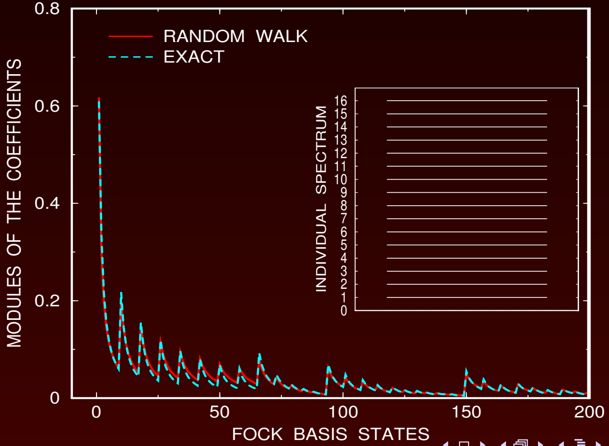
Stochastic vs. Quantum Occupation Probabilities

- Zooming in the previous spectrum for $p = 12$ and $n = 24$



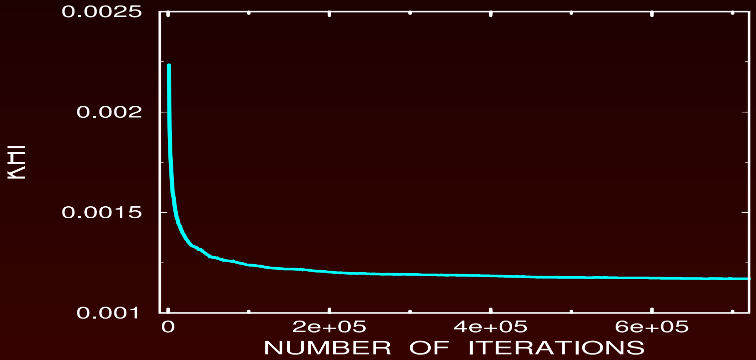
Stochastic vs. Quantum Occupation Probabilities

- 16 particles on 32 levels ($\mathcal{N}_{it} = 300\ 000$ iterations)
  Fock space dimension $\mathcal{N}(32/16) = 601\ 080\ 390$



Stochastic vs. Quantum Occupation Probabilities

- 16 particles on 32 levels; ground-state wave-function $\longrightarrow L = 1$



$$\chi = \left[\frac{1}{N-1} \sum_{K=1}^{N} \left(|C^{q}_{1,K}| - |C^{s}_{1,K}| \right)^2 \right]^{1/2}$$

Stochastic Approach: Problem with Excited States?

- So far we have considered the ground-state wave functions

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$$\mathcal{P} \sim |C|^2 \leftrightarrow |C|$$

so there was no problem to obtain the wave-function out of $|C_{1,K}|^2$

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- We arrive at the problem: The wave-function <u>of the excited states</u> cannot be obtained in the same way ...

Extending the Random Walk: Excited States

- We consider again the full ensemble of the Fock-basis vectors

$$\{|\phi_K\rangle;\ K = 1,\, 2,\, 3,\ \ldots\ \mathcal{N}_b\}$$

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- Next we construct the whole series of the random walk processes by beginning with $|\Phi_2>$, $|\Phi_3>$, ...

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- ... but now: how should we compare the stochastic results with the quantum case?

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- ... but now: how should we compare the stochastic results with the quantum case?

- The random walk algorithm provides neither the signs of the $C-$coefficients - nor the energies ...

Extending the Random Walk: Excited States (II)

- Consider a set of linearly independent vectors $\{|\Psi_L\rangle\}$. We will orthonormalise them, beginning with $|\Psi_1>$ as follows:

– We normalise $|\Psi_1>$: $|\Psi_1\rangle \rightarrow |\Theta_1\rangle = \frac{1}{||\,\Psi_1\,||}|\Psi_1\rangle$

– We subtract the parallel part of $|\Psi_2>$ from $|\Theta_1>$

$$|\Psi_2\rangle \rightarrow |\Psi_2'\rangle = |\Psi_2\rangle - \;(<\Theta_1|\Psi_2>)\;|\Theta_1\rangle$$

- We normalise this last vector:

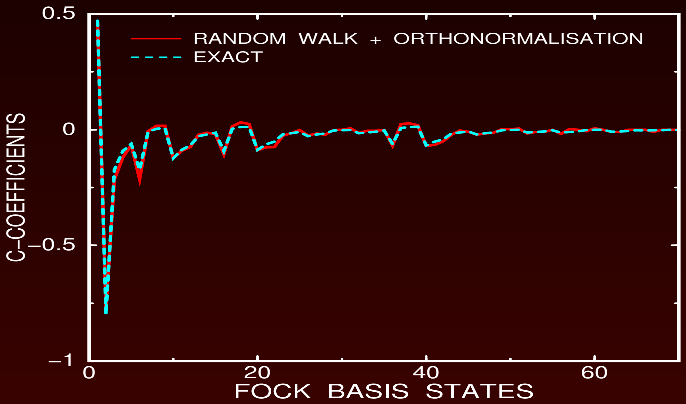
$$|\Psi_2'\rangle \rightarrow |\Theta_2\rangle = \frac{1}{||\,\Psi_2\,||}\,|\Psi_2\rangle$$

- We subtract the parallel part of $|\Psi_2>$ from $|\Theta_1>$ and $|\Theta_2>$

$$|\Psi_3'\rangle \rightarrow |\Psi_3\rangle - \langle\Theta_1|\Psi_3>\;\;|\Theta_1\rangle - \langle\Theta_2|\Psi_3>\;\;|\Theta_2>$$

Orthonormalisation Scheme - Illustration

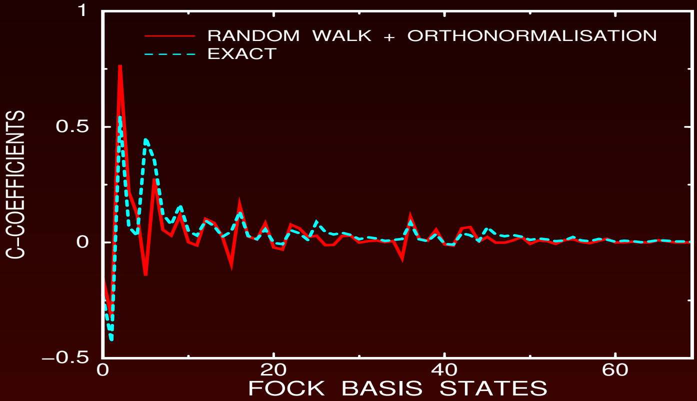
- 8 particles on 16 levels - 1^{rst} excited state



... and apparently we are able to obtain *the wave function of an excited state*. However:

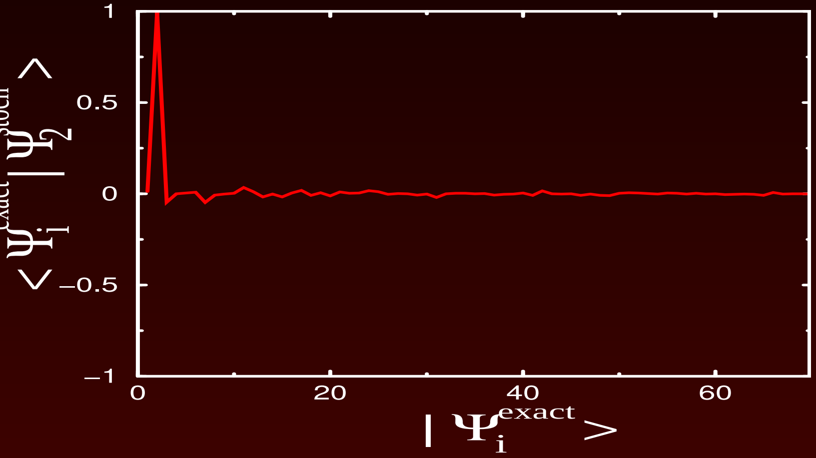
Orthonormalisation Scheme - Illustration

- 8 particles on 16 levels - 2^{nd} excited state

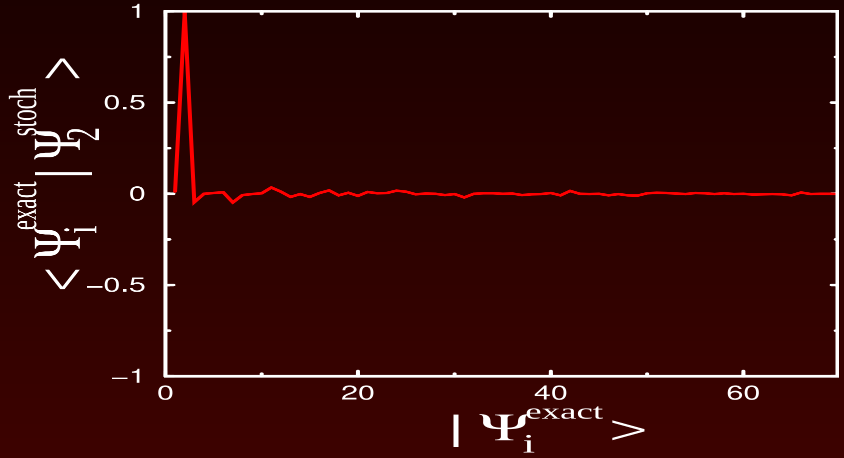


... and *apparently* the scheme does not seem to perform well for yet another excited state ... Is it a real problem?

Overlaps: Stochastic vs. Exact



Overlaps: Stochastic vs. Exact



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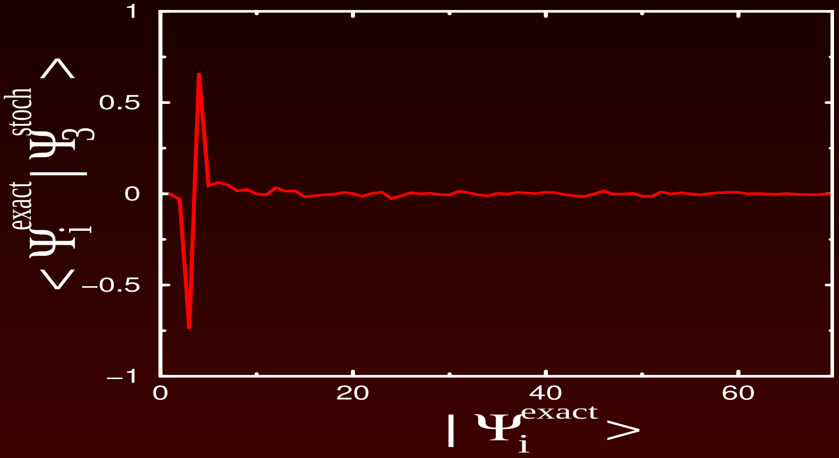

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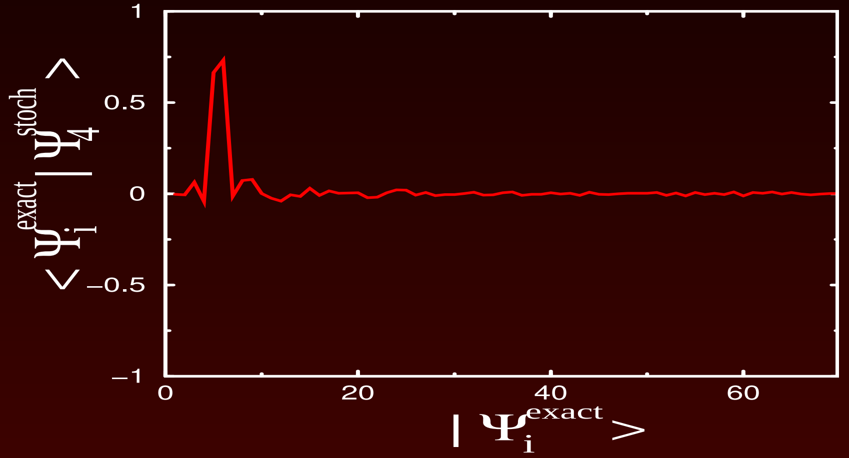

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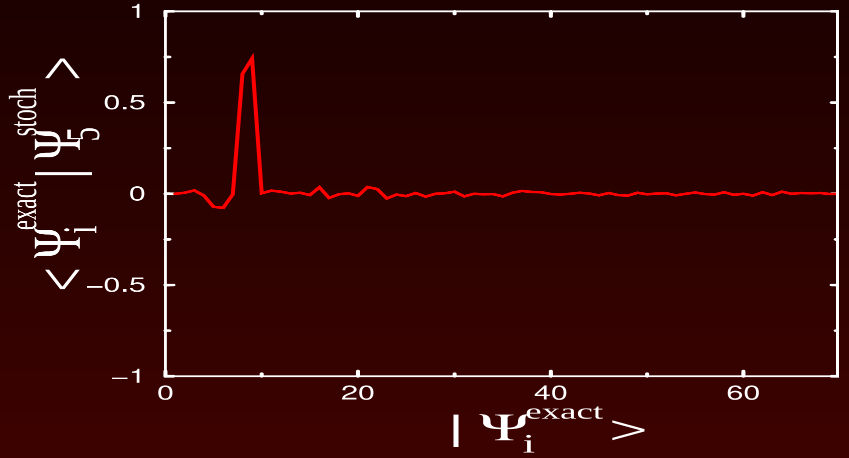

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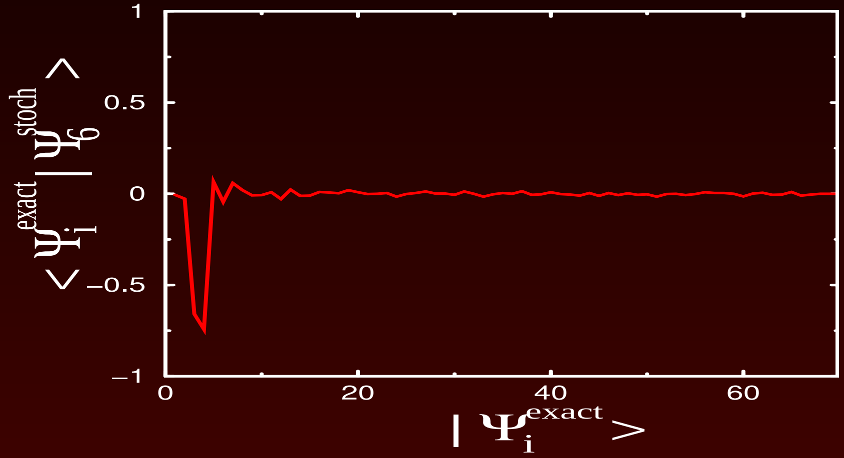

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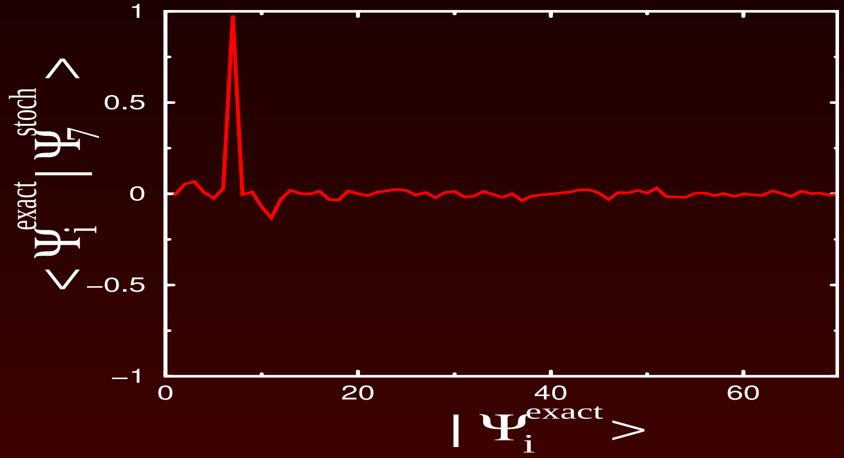

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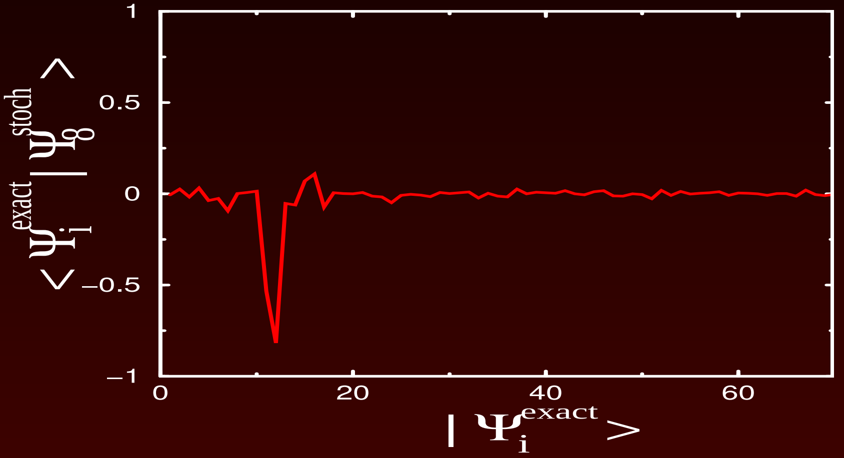

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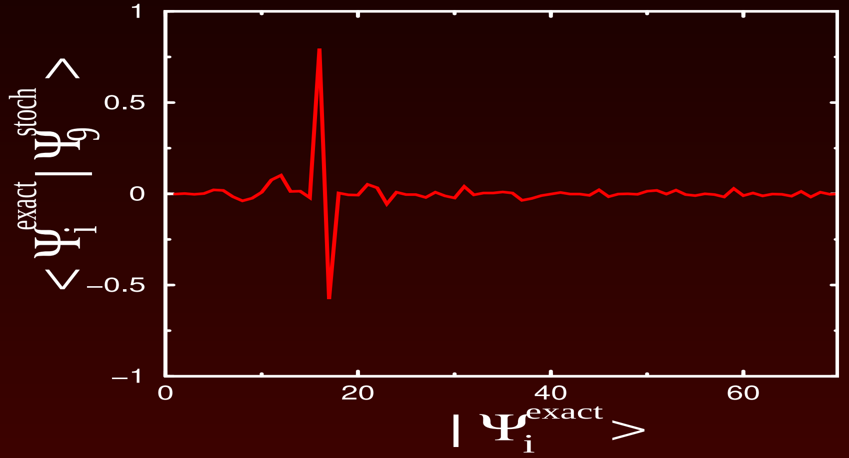


Observations, Interpretation, Partial Conclusions

• We just have observed that the *quantum* and *stochastic* Fock-basis vectors are similar - but not identical

• More precisely: some stochastic vectors have more than 99% of overlap with *one* of their quantum partners ...

• ... some others have a strong overlap with ~ 2 quantum partners, and several 'tiny' overlaps with the others

• Observation: the stochastic basis vectors seem to be often nearly parallel to their quantum partners; sometimes they rather lie in a two-dimensional hyperplane

• Clearly the stochastic and quantum Fock bases are not *identical*;

Are they equivalent i.e. differing by an orthogonal transformation?

Certain Property of Eigenvectors

- Let us consider again a Fock basis $\{|\Phi_K\rangle;\ K = 1 \ldots N_b\}$
- Eigenvalues and eigenvectors of $\hat{H}_1$ in the Fock space obey:

$$\hat{H}_1\ |\Phi_N\rangle = \mathcal{E}_N\ |\Phi_N\rangle \quad \text{with} \quad \mathcal{E}_N = \sum_{\alpha \in \{Conf.\}_N} e_\alpha$$

- Eigenvectors $|\Psi_J\rangle$ satisfy: $|\Psi_J\rangle = \sum_{K=1}^{N_b} C_{JK}|\Phi_K\rangle$
- Eigenvalues of $\hat{H}$ can be calculated knowing the $\{\mathcal{E}_L\}$ energies:

$$E_J = \sum_{L=1}^{N_b} C_{JL}^2 \mathcal{E}_L + \sum_{L,M=1}^{N_b} C_{JL} C_{JM} \langle \Phi_L | \hat{H}_2 | \Phi_M \rangle$$

- Knowing coefficients C_{JL} from the stochastic simulation, we orthonormalise the vectors $\longrightarrow$ verify whether they give eigenenergies!

The Eigenvalues of $\hat{\mathrm{H}}$ and Stochastic Features

- Denoting by n the number of nucleons, we have

$$\langle \Phi_L | \hat{H}(2) | \Phi_M \rangle = \begin{cases} -\frac{1}{2}\, n\, |G| & \text{if } M = L, \\ -|G| & \text{if } M \neq L, \text{ but } |\Phi_M\rangle \text{ and } |\Phi_L\rangle \\ & \text{differ by one exited pair,} \\ \;0 & \text{otherwise} \end{cases}$$

- We express unknown eigenenergies by stochastic coefficients

$$E_J = \sum_L \Big[\, C_{JL}^2 (\mathcal{E}_L - \tfrac{1}{2}\, n\, |G|) - \; C_{JL}\, |G| \sum_{\delta L} C_{J,L+\delta L} \,\Big]\;;$$

the symbol $\{L + \delta L\}$ refers to configurations that differ from those denoted $\{L\}$ by one excited pair

The Eigenvalues of $\hat{\mathrm{H}}$ and Stochastic Features

p=8 particles on n=16 levels - Error

Fock space $\mathcal{N}$ = 12 870

EXACT [MeV]	RANDOM WALK [MeV]	RELATIVE ERROR
16.8891704	16.9120315	0.14%
19.4809456	19.5437517	0.32%
21.4463235	21.5163029	0.33%
21.4463235	21.5187773	0.34%
23.4307457	23.4899241	0.25%
23.4307457	23.4963815	0.28%
23.7797130	23.9403046	0.67%
25.4418890	25.4581811	0.06%
25.4418890	25.4605459	0.07%
25.6148968	25.6849886	0.27%
25.8221082	25.9242843	0.40%
25.8221082	25.9578009	0.52%
27.8143803	27.8793481	0.23%
27.8143803	27.8875293	0.26%
...	...	...

The Eigenvalues of $\hat{\mathrm{H}}$ and Stochastic Features

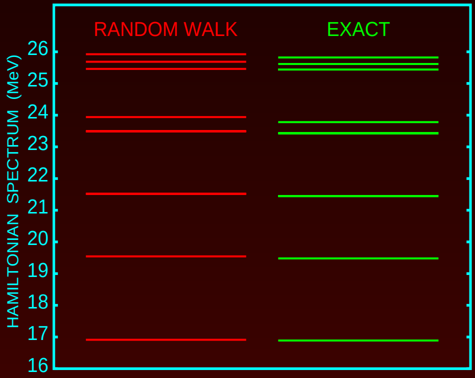
12 particles on 24 levels - Error

Fock space $\mathcal{N} = 2\ 704\ 156$

EXACT [MeV]	RANDOM WALK [MeV]	RELATIVE ERROR
36.8391727	36.8981242	0.16%
39.9047355	40.0512103	0.37%
41.7482282	41.8456965	0.23%
41.7482282	41.8521919	0.25%
43.6532878	43.7391981	0.20%
43.6532878	43.7438472	0.21%
44.3047857	44.4975191	0.43%
45.5945444	45.6720849	0.17%
45.5945444	45.6788884	0.18%
45.9368443	46.0291365	0.20%
46.3210968	46.4902340	0.37%
46.3210968	46.5009797	0.40%
47.5618469	47.6218935	0.13%
...	...	...

The Eigenvalues of $\hat{\mathrm{H}}$ and Stochastic Features

8 particles on 16 levels - the first 11 levels



The Eigenvalues of $\hat{\mathrm{H}}$ and Stochastic Features

8 particles on 16 levels - the first 33 levels

The Eigenvalues of $\hat{\mathrm{H}}$ and Stochastic Features

8 particles on 16 levels - All levels

The Eigenvalues of $\hat{\mathrm{H}}$ and Stochastic Features

12 particles on 24 levels - the first 25 levels

Question of the 'Universal Probability Distribution'

- The results presented above were obtained by using, as a working hypothesis, the following form of the parametrisation of the transition probability:

$$\mathbf{P}_{\alpha\to\beta} = \frac{\mathbf{K}_\alpha}{\mathbf{a}\,(\Delta\mathcal{E}_{\alpha\beta})^2 + \mathbf{b}\;\Delta\mathcal{E}_{\alpha\beta} + \mathbf{c}}$$

where

$$\Delta\mathcal{E}_{\alpha\beta} = |\mathcal{E}_\alpha - \mathcal{E}_\beta|$$

and where K_α is a normalisation constant; a, b and c are adjustable parameters.

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• We have constructed the solutions to the Schrödinger equation by using the totally independent random walk (Markov chain) concepts

• The eigen-energies constructed using the random walk simulations agree within a few permille level with the exact ones

• Stochastic solutions are systematically higher than the exact ones

Summary

- We discussed the problem of the nuclear pairing Hamiltonian written down in the Fock space representation (for $\mathcal{N} \sim 10^{40}$ spaces)

- We obtained the exact results using the so-called P_1, P_2 and P_{12} symmetries and the Lanczos diagonalisation technique

- We have constructed the solutions to the Schrödinger equation by using the totally independent random walk (Markov chain) concepts

- The eigen-energies constructed using the random walk simulations agree within a few permille level with the exact ones

- Stochastic solutions are systematically higher than the exact ones

- The Lanczos approach has a natural limitations related to the present-day computer memory; *the stochastic simulation is extremely fast and can go in principle 'up to infinity'*

Comments and Conclusions

• The Lanczos approach has a natural limitations related to the present-day computer memory; *the stochastic simulation is extremely fast and can go in principle 'up to infinity'*

• We would like to perform more detailed tests of the structure of the 'universal probability' distribution

• The fact that such a probability distribution seems to exist, acting the same way independently of the structure of the Fock-space states looks to us of extreme importance

• The (small) discrepancies with respect to the exact solutions can be due to the inaccuracies of the elementary probability distribution and/or to a 'small non-Markovian corrections'