Munich University of Technology

Centre for Mathematical Sciences

- Bachelor Thesis -

The Representability Problem in Many-Body Quantum Mechanics

by

Christian Mendl (christian_mendl@web.de)

Supervisor: Prof. Ph.D. Gero Friesecke
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Declaration of Authorship

I hereby declare that the work presented here is original and the result of my own investigations, except as acknowledged.

Garching, 24th October 2006 ....

Christian Mendl

Contents

1 Introduction

As a recurring scheme in many-particle quantum mechanics, one observes that the Hamiltonian H contains at most two-particle interactions, e.g. the Coulomb repulsion of electrons. That is, although there is an arbitrary large number N of electrons, the total energy of the system can be calculated from the kinetic energy of each electron (plus the contribution of a fixed external potential), and the interaction potential between electron pairs. This can be exploited by rewriting the expected value of an N-fermion state Ψ as

$$\langle \Psi \mid H\Psi \rangle = \operatorname{trace}\left(h\Gamma_\Psi\right), \tag{1}$$

where the "two-body operator" h describes the interaction and Γ_Ψ is the two-body reduced density matrix of Ψ. Note that the right side is linear in Γ_Ψ, and h operates on the two-body space, whereas H is an N-body operator. Thus, the ground state of the system can be found by solving a linear programming problem on the set of N-representable two-body density matrices instead of a quadratic minimization problem for N-fermion states. This motivates the "representability problem":

Give a "practical" characterization of the set of 2-body reduced density matrices derived from N-fermion wave functions.

The Pauli exclusion principle states that the total wave function must be antisymmetric, a crucial property which contributes most to the difficulties. Although reduced density matrices were extensively studied by, for example, C.N. Yang [3], A.J. Coleman [5] and P.-O. Löwdin, no result of definite importance has yet been obtained.

In the following chapter we give the basic definitions and derive equation (1). The next section contains a collection of properties of one- and two-body density matrices. Afterwards conjectures and further ideas are presented. A detailed appendix explains preliminary concepts used in many-particle quantum mechanics.

2 Basic Definitions

We always assume that $\mathcal{H}$ is a finite-dimensional or separable Hilbert space. By $\wedge^N \mathcal{H}$ we denote the antisymmetrized N-fold tensor product (see Standard Example 23 in the appendix).

Definition 1. *Let $\Psi \in \wedge^N \mathcal{H}$, $\|\Psi\| = 1$, then its* p-body reduced density matrix γ_Ψ^p *($1 \leq p \leq N$) is a linear continuous operator $\wedge^p \mathcal{H} \to \wedge^p \mathcal{H}$ given by*

$$\langle \chi \mid \gamma_\Psi^p \phi \rangle := \langle a_\phi \Psi \mid a_\chi \Psi \rangle = \left\langle \Psi \mid a_\phi^\dagger a_\chi \Psi \right\rangle \quad \forall\, \phi, \chi \in \wedge^p \mathcal{H},$$

where $a_\phi^\dagger$ *and* a_χ *are the creation and annihilation operators of the states* ϕ *and* χ*, respectively. We denote the* one- and two-body density matrices *by* $\gamma_\Psi := \gamma_\Psi^1$ *and* $\Gamma_\Psi := \gamma_\Psi^2$.

The integral version of the creation and annihilation operators for L^2 spaces (given in the appendix) allows us to identify γ_Ψ^p as an integral operator: for all $\phi \in \wedge^p\mathcal{H}$,

$$\left(\gamma_\Psi^p\phi\right)(x_1,\ldots,x_p) = \int_{\Omega^p} \gamma_\Psi^p(x_1,\ldots,x_p,x'_1,\ldots,x'_p)\,\phi(x'_1,\ldots,x'_p)\,\mathrm{d}x'_1\ldots\,\mathrm{d}x'_p$$

with the integral kernel (also denoted by γ_Ψ^p)

$$\begin{aligned}\gamma_\Psi^p(x_1,\ldots,x_p,&x'_1,\ldots,x'_p) :=\\ &\binom{N}{p}\int_{\Omega^{N-p}} \Psi(x_1,\ldots,x_p,x_{p+1},\ldots,x_N)\\ &\times\overline{\Psi(x'_1,\ldots,x'_p,x_{p+1},\ldots,x_N)}\,\mathrm{d}x_{p+1}\ldots\,\mathrm{d}x_N.\end{aligned}$$

Thus we can state the following

Theorem 2. γ_Ψ^p *is compact, self-adjoint, nonnegative, trace class and has trace*

$$\operatorname{trace}\gamma_\Psi^p = \int_{\Omega^p}\gamma_\Psi^p(x_1,\ldots,x_p,x_1,\ldots,x_p)\,\mathrm{d}x_1\ldots\,\mathrm{d}x_p = \binom{N}{p}.$$

Proof. γ_Ψ^p is positive semidefinite as

$$\langle\phi\,|\,\gamma_\Psi^p\phi\rangle = \|a_\phi\Psi\|^2 \geq 0 \quad \forall\phi\in\wedge^p\mathcal{H}.$$

The other assertions follow from the properties of integral operators given in the appendix. □

Assuming that the linear, self-adjoint Schrödinger operator H contains only one- and two-body interactions, it can be rewritten as

$$H = \sum_{\alpha<\beta} h_{\alpha,\beta}$$

for some $h : \wedge^2\mathcal{H} \to \wedge^2\mathcal{H}$. Given a complete orthonormal system $(\phi_i)_i$ in $\wedge^2\mathcal{H}$, in terms of Second Quantization,

$$H = \sum_{i,j}\langle\phi_i\,|\,h\phi_j\rangle\,a_{\phi_i}^\dagger a_{\phi_j}.$$

Now we gain equation 1: for all normalized $\Psi \in \wedge^N \mathcal{H}$,

$$\begin{aligned} \langle \Psi \,|\, H\Psi \rangle &= \sum_{i,j} \langle \phi_i \,|\, h\phi_j \rangle \left\langle \Psi \,|\, a^\dagger_{\phi_i} a_{\phi_j} \Psi \right\rangle \\ &= \sum_{i,j} \langle \phi_i \,|\, h\phi_j \rangle \langle \phi_j \,|\, \Gamma_\Psi \phi_i \rangle \\ &= \sum_{i} \langle \phi_i \,|\, h\Gamma_\Psi \phi_i \rangle = \operatorname{trace}\left(h\Gamma_\Psi \right). \end{aligned}$$

An immediate consequence is the following formula for the ground state energy:

Proposition 3. *Let H be given as above, then*

$$\begin{aligned} \inf \operatorname{spec} H &= \inf \left\{ \langle \Psi \,|\, H\Psi \rangle \mid \Psi \in \wedge^N \mathcal{H},\ \|\Psi\| = 1 \right\} \\ &= \inf \left\{ \operatorname{trace}\left(h\Gamma_\Psi \right) \mid \Psi \in \wedge^N \mathcal{H},\ \|\Psi\| = 1 \right\}, \end{aligned}$$

i.e. the ground state energy can be found by minimizing over the set of N-representable two-body density matrices.

Note that for the minimization problem, it is sufficient to characterize the set

$$\overline{\operatorname{conv} \{ \Gamma_\Psi \mid \Psi \in \wedge^N \mathcal{H},\ \|\Psi\| = 1 \}}^{\|\cdot\|_{\text{trace}}}.$$

To illustrate the complexity reduction, let $\dim \mathcal{H} =: K < \infty$ and compare the following estimations for the degrees of freedom:

$$\begin{aligned} \Gamma_\Psi \in L\left(\wedge^2 \mathcal{H} \right) &\to \mathbb{C}^{\binom{K}{2}^2} \sim \mathbb{C}^{K^4}, \quad \text{whereas} \\ \Psi \in \wedge^N \mathcal{H} &\to \mathbb{C}^{\binom{K}{N}} \sim \mathbb{C}^{K^N}. \end{aligned}$$

3 Properties of Fermion Density Matrices

By the Hilbert Schmidt theorem, there is a complete orthonormal system $(\phi_i)_i$ in $\wedge^p \mathcal{H}$ of eigenvectors of γ^p_Ψ, i.e.

$$\gamma^p_\Psi \phi_i = \lambda_i \phi_i, \quad \lambda_i \in \mathbb{R} \qquad \text{for all } i.$$

Consider the one-body case $p = 1$. By Standard Example 23 in the appendix, Ψ can be expanded in $(\phi_{i_1} \wedge \cdots \wedge \phi_{i_N})_{i_1 < \cdots < i_N}$. The following proposition shows that it is sufficient to consider eigenvectors with nonzero eigenvalues only, which will be particularly interesting if $\operatorname{rank} \gamma_\Psi < \infty$.

Proposition 4. *Ψ can be expanded as a linear combination of Slater determinants constructed from eigenvectors of γ_Ψ which belong to nonzero eigenvalues.*

Proof. What remains to be shown is the following: if $\gamma_\Psi \phi_i = 0$, ϕ_i won't show up in the expansion:

$$\|a_{\phi_i}\Psi\|^2 = \langle \phi_i \,|\, \gamma_\Psi \phi_i \rangle = 0.$$

□

Note that γ_Ψ^p contains less information the smaller p gets, or more strictly speaking:

Proposition 5. *Let $\Psi \in \wedge^N \mathcal{H}$, $\|\Psi\| = 1$, then γ_Ψ^p can be obtained from γ_Ψ^{p+1}.*

Proof. For any complete orthonormal system $|i\rangle_i$ of $\mathcal{H}$,

$$\begin{aligned}
&\sum_k \left\langle i_1 \wedge \cdots \wedge i_p \wedge k \,|\, \gamma_\Psi^{p+1}\, j_1 \wedge \cdots \wedge j_p \wedge k \right\rangle \\
&= \left\langle \Psi \,|\, a_{j_1}^\dagger \cdots a_{j_p}^\dagger \left(\sum_k \hat{n}_k \right) a_{i_p} \cdots a_{i_1} \Psi \right\rangle \\
&= (N-p) \left\langle i_1 \wedge \cdots \wedge i_p \,|\, \gamma_\Psi^p\, j_1 \wedge \cdots \wedge j_p \right\rangle .
\end{aligned}$$

□

Proposition 6. *Let $\Psi := \psi_1 \wedge \cdots \wedge \psi_N$ be a Slater determinant with orthonormal $\psi_1, \ldots, \psi_N \in \mathcal{H}$. Then γ_Ψ^p is the orthogonal projection on the subspace spanned by $\left(\psi_{i_1} \wedge \cdots \wedge \psi_{i_p}\right)_{i_1 < \cdots < i_p}$.*

This can be seen by an explicit calculation or derived directly from the definition of γ_Ψ^p using creation and annihilation operators.

It is currently not known whether the converse is also true, except for $p = 1$:

Proposition 7. *Ψ is a Slater determinant iff γ_Ψ is an orthogonal projection.*

Proof. Only "$\Leftarrow$" remains to be shown. From $\sigma(\gamma_\Psi) = \{0, 1\}$ and $\operatorname{trace} \gamma_\Psi = N$ it follows that $\operatorname{rank} \gamma_\Psi = N$. That is, by proposition 4, Ψ can be expanded into a single Slater determinant. □

We make use of the anticommutator relations for creation and annihilation operators to show the following proposition, which is intricately connected with the antisymmetry constraint of the wave function.

Proposition 8. *The expected values of* γ_Ψ *are in the range* $[0,1]$.

Proof. We have already shown that γ_Ψ is positive semidefinite. $\gamma_\Psi \le 1$ follows from

$$\langle \phi \,|\, \gamma_\Psi \phi \rangle = \left\langle \Psi \,|\, a_\phi^\dagger a_\phi \Psi \right\rangle = \left\langle \Psi \,|\, \left(1 - a_\phi a_\phi^\dagger\right) \Psi \right\rangle = \|\Psi\|^2 - \left\| a_\phi^\dagger \Psi \right\|^2 \le 1.$$

□

We state a classification of the ranks of fermion one-body density matrices. A proof can be found in [4].

Theorem 9. *There exists a* $\Psi \in \wedge^N \mathcal{H}$ *such that* $\operatorname{rank} \gamma_\Psi = K$, *if and only if*

$$K = \begin{cases} 1 & N = 1 \\ \ge 2, \ \textit{even} & N = 2 \\ \ge N, \ne N+1 & N \ge 3 \end{cases}$$

In particular, $\operatorname{rank} \gamma_\Psi$ *is at least* N *and cannot be equal to* $N+1$.

Given an unitary operator $U : \mathcal{H} \to \mathcal{H}$, we obtain an unitary operator (also denoted by U) acting on $\wedge^N \mathcal{H}$ by

$$U\left(i_1 \wedge \cdots \wedge i_N\right) := \left(U i_1\right) \wedge \cdots \wedge \left(U i_N\right).$$

Proposition 10. *Given such an unitary operator* U,

$$U^* \gamma_{U\Psi}^p U = \gamma_\Psi^p.$$

Proof. We use

$$U^* a_{U\phi}^\dagger U = a_\phi^\dagger, \quad U^* a_{U\phi} U = a_\phi^\dagger \qquad \text{for all } \phi \in \wedge^N \mathcal{H}$$

to get

$$\begin{aligned} \langle \chi \,|\, U^* \gamma_{U\Psi}^p U \phi \rangle &= \left\langle U\Psi \,|\, a_{U\phi}^\dagger a_{U\chi} U \Psi \right\rangle = \left\langle \Psi \,|\, \left(U^* a_{U\phi}^\dagger U\right) \left(U^* a_{U\chi} U\right) \Psi \right\rangle \\ &= \left\langle \Psi \,|\, a_\phi^\dagger a_\chi \Psi \right\rangle = \langle \chi \,|\, \gamma_\Psi^p \phi \rangle \quad \text{for all } \phi, \chi \in \wedge^p \mathcal{H}. \end{aligned}$$

□

This might be a starting point for a simplification of the problem: introduce equivalence classes on $\wedge^N \mathcal{H}$ by $\Psi \sim \Phi :\Leftrightarrow \Psi = U\Phi$ for some unitary U.

As an immediate consequence of proposition 10, the convex hull

$$\operatorname{conv}\left\{\gamma_\Psi^p \,|\, \Psi \in \wedge^N \mathcal{H}, \|\Psi\| = 1\right\}$$

is invariant under these unitary transformations, since

$$U^* \left(\sum_{i=1}^n \alpha_i \gamma_{\Psi_i}^p\right) U = \sum_{i=1}^n \alpha_i \gamma_{U^*\Psi_i}^p$$

for all $0 \leq \alpha_1, \ldots, \alpha_n \leq 1$ with $\alpha_1 + \cdots + \alpha_n = 1$.

3.1 Duality between γ_Ψ^p and γ_Ψ^{N-p}

We may further expand the concept of the annihilation operator: define an antilinear operator

$$\hat{\Psi} : \wedge^p \mathcal{H} \to \wedge^{N-p} \mathcal{H}, \quad (\hat{\Psi}\phi)(x) := (a_\phi \Psi)(x) = \binom{N}{p}^{\frac{1}{2}} \int_{\Omega^p} \overline{\phi(y)} \Psi(y, x) \,\mathrm{d}y,$$

where $x \in \Omega^{N-p}$ and y runs over all Ω^p. Note that for all $\phi \in \wedge^p \mathcal{H}$ and $\chi \in \wedge^{N-p} \mathcal{H}$,

$$\begin{aligned}
\left\langle \chi \,|\, \hat{\Psi}\phi \right\rangle &= \binom{N}{p}^{\frac{1}{2}} \int_{\Omega^N} \overline{\chi(x)\phi(y)} \Psi(y, x) \,\mathrm{d}x \,\mathrm{d}y \\
&= (-1)^{(N-p)\,p} \binom{N}{p}^{\frac{1}{2}} \int_{\Omega^N} \overline{\phi(y)\chi(x)} \Psi(x, y) \,\mathrm{d}x \,\mathrm{d}y \\
&= (-1)^{(N-p)\,p} \left\langle \phi \,|\, \hat{\Psi}\chi \right\rangle,
\end{aligned}$$

where the sign factor comes from the permutation $(y, x) \to (x, y)$. Using this property, it follows that

$$\langle \chi \,|\, \gamma_\Psi^p \phi \rangle = \langle a_\phi \Psi \,|\, a_\chi \Psi \rangle = \left\langle \hat{\Psi}\phi \,|\, \hat{\Psi}\chi \right\rangle = (-1)^{(N-p)\,p} \left\langle \chi \,|\, \hat{\Psi}^2 \phi \right\rangle$$

for all $\phi, \chi \in \wedge^p \mathcal{H}$, i.e.

$$\gamma_\Psi^p = (-1)^{(N-p)\,p} \,\hat{\Psi}^2.$$

Proposition 11. *There is a one-to-one correspondence between the normalized eigenvectors of γ_Ψ^p and γ_Ψ^{N-p} with the same nonzero eigenvalue.*

Proof. Let

$$\gamma_\Psi^p \phi = \lambda\phi, \quad \lambda > 0, \quad \phi \in \wedge^p \mathcal{H} \text{ with } \|\phi\| = 1.$$

Define

$$\chi := \frac{i^{(N-p)\,p}}{\sqrt{\lambda}} \hat{\Psi}\phi,$$

then $\|\chi\| = 1$ as

$$\left\|\hat{\Psi}\phi\right\|^2 = \|a_\phi \Psi\|^2 = \langle \phi \,|\, \gamma_\Psi^p \phi\rangle = \lambda \langle \phi \,|\, \phi \rangle$$

and χ is an eigenvector of γ_Ψ^{N-p} with eigenvalue λ. In fact,

$$\gamma_\Psi^{N-p}\left(\hat{\Psi}\phi\right) = (-1)^{(N-p)\,p}\hat{\Psi}^3\phi = \hat{\Psi}\gamma_\Psi^p\phi = \lambda\left(\hat{\Psi}\phi\right).$$

Applying the same rule to χ, we recover the original ϕ:

$$\frac{i^{p\,(N-p)}}{\sqrt{\lambda}}\hat{\Psi}\chi = \frac{(-1)^{p\,(N-p)}}{\lambda}\hat{\Psi}^2\phi = \frac{1}{\lambda}\gamma_\Psi^p\phi = \phi.$$

If $\phi' \in \wedge^p\mathcal{H}$ is another normalized eigenvector of λ perpendicular to ϕ, then χ' is perpendicular to χ:

$$\langle \chi' \,|\, \chi \rangle = \frac{1}{\lambda}\left\langle \hat{\Psi}\phi' \,|\, \hat{\Psi}\phi \right\rangle = \frac{1}{\lambda}\langle \phi \,|\, \gamma_\Psi^p \phi' \rangle = \langle \phi \,|\, \phi' \rangle = 0.$$

Note that γ_Ψ^p is Hilbert-Schmidt, hence all nonzero eigenvalues have finite multiplicity and eigenvectors corresponding to different eigenvalues are orthogonal. □

3.2 Decomposition of the One-Body Density Matrix

We first derive a formula due to Ando [2]. Let $|i\rangle_i$ be a complete orthonormal system of eigenvectors of γ_Ψ with corresponding eigenvalues λ_i such that λ_1 is the greatest eigenvalue. Ψ can be expanded in Slater determinants as follows:

$$\Psi = \sum_{\substack{I=(i_1,\ldots,i_N)\\ i_1<\cdots<i_N}} x_I\,|i_1,\ldots,i_N\rangle, \quad x_I \in \mathbb{C}.$$

Set

$$\Phi_a := \sum_{1\in I} x_I\,|i_2,\ldots,i_N\rangle \in \wedge^{N-1}\mathcal{H} \quad \text{and}$$

$$\Phi_b := \sum_{1\notin I} x_I\,|i_1,\ldots,i_N\rangle \in \wedge^{N}\mathcal{H},$$

then $\Psi = a_1^\dagger \Phi_a + \Phi_b$. From that,

$$\langle i \,|\, \gamma_\Psi j \rangle = \left\langle \Psi \,|\, a_j^\dagger a_i \Psi \right\rangle = \left\langle \Phi_a \,|\, a_1 a_j^\dagger a_i a_1^\dagger \Phi_a \right\rangle$$
$$+ \left\langle \Phi_b \,|\, a_j^\dagger a_i a_1^\dagger \Phi_a \right\rangle + \left\langle \Phi_a \,|\, a_1 a_j^\dagger a_i \Phi_b \right\rangle + \left\langle \Phi_b \,|\, a_j^\dagger a_i \Phi_b \right\rangle .$$

Since $a_1 \Phi_a = 0$, the first term equals

$$\left\langle \Phi_a \,|\, a_1 a_j^\dagger a_i a_1^\dagger \Phi_a \right\rangle = \|\Phi_a\|^2 \langle i \,|\, 1 \rangle \langle 1 \,|\, j \rangle + \left\langle \Phi_a \,|\, a_j^\dagger a_i \Phi_a \right\rangle ,$$

and

$$\|\Phi_a\|^2 = \langle 1 \,|\, \gamma_\Psi 1 \rangle = \lambda_1 .$$

Iff $\Phi_b = 0$, we have $\lambda_1 = \|\Phi_a\|^2 = \|\Psi\|^2 = 1$; then

$$\gamma_\Psi = |1\rangle \langle 1| + \gamma_{\Phi_a} .$$

Now, let $\lambda_1 \neq 1$, i.e. $\lambda_1 < 1$.

Clearly, $\left\langle \Phi_a \,|\, a_1 a_j^\dagger a_i \Phi_b \right\rangle$ is zero for $i = 1$ and $i, j \neq 1$. In the remaining case $i \neq 1, j = 1$ it equals $\langle i \,|\, \gamma_\Psi 1 \rangle = 0$, i.e. it vanishes altogether. Note that this implies the total orthogonality of Φ_a and Φ_b, $\langle \Phi_a \,|\, a_i \Phi_b \rangle = 0$ for all i. An analogous argument shows that $\left\langle \Phi_b \,|\, a_j^\dagger a_i a_1^\dagger \Phi_a \right\rangle = 0$ for all i, j.

Set

$$\Psi_a := \frac{\Phi_a}{\|\Phi_a\|} \quad \text{and} \quad \Psi_b := \frac{\Phi_b}{\|\Phi_b\|},$$

then the decomposition can be written as

$$\langle i \,|\, \gamma_\Psi j \rangle = \lambda_1 \langle i \,|\, 1 \rangle \langle 1 \,|\, j \rangle + \lambda_1 \langle i \,|\, \gamma_{\Psi_a} j \rangle + \|\Phi_b\|^2 \langle i \,|\, \gamma_{\Psi_b} j \rangle .$$

Using

$$N = \operatorname{trace} \gamma_\Psi = \sum_i \langle i \,|\, \gamma_\Psi i \rangle = \lambda_1 + \lambda_1 (N-1) + N \|\Phi_b\|^2 ,$$

we get $\|\Phi_b\|^2 = 1 - \lambda_1$. Summarising finally yields

Lemma 12. γ_Ψ *can be decomposed into*

$$\gamma_\Psi = \lambda_1 |1\rangle \langle 1| + \lambda_1 \gamma_{\Psi_a} + (1 - \lambda_1) \gamma_{\Psi_b}, \tag{2}$$

where $\Psi_a \in \wedge^{N-1} \mathcal{H}$ *and* $\Psi_b \in \wedge^N \mathcal{H}$ *are normalized functions such that*

$$\Psi = \sqrt{\lambda_1} \cdot a_1^\dagger \Psi_a + \sqrt{1 - \lambda_1} \cdot \Psi_b \quad \textit{and}$$
$$a_1 \Psi_a = 0, \quad a_1 \Psi_b = 0, \quad \langle \Psi_a \,|\, a_i \Psi_b \rangle = 0 \quad \forall\, i.$$

In the following we need another lemma which can be found in [2].

Lemma 13. *In the decomposition* (2)*, if* γ_{Ψ_a} *has a normalized eigenvector* ϕ *belonging to the eigenvalue* 1*, then* ϕ *will also be an eigenvector of* γ_Ψ *belonging to the eigenvalue* λ_1*, and* $a_\phi \Psi_b = 0$ *when* $\lambda_1 \neq 1$*.*

Proof. Since λ_1 is the greatest eigenvalue of γ_Ψ, the assertion follows from

$$\lambda_1 \geq \langle \phi \,|\, \gamma_\Psi \phi \rangle = \lambda_1 \left| \langle 1 \,|\, \phi \rangle \right|^2 + \lambda_1 \underbrace{\langle \phi \,|\, \gamma_{\Psi_a} \phi \rangle}_{=1} + (1 - \lambda_1) \langle \phi \,|\, \gamma_{\Psi_b} \phi \rangle \geq \lambda_1.$$

□

Now we can proof a slightly sharper form of a result due to Ando [2]. Proposition 7 handles the case $\operatorname{rank} \gamma_\Psi = N$, and $\operatorname{rank} \gamma_\Psi$ can never be $N+1$, by theorem 9. The next simplest step is therefore rank $N+2$.

Proposition 14. *Let* $\operatorname{rank} \gamma_\Psi = N + 2$*. Then,*

- *if* N *is odd,* $\lambda_1 = 1$ *and each of the remaining nonzero eigenvalues will be evenly degenerate,*
- *if* N *is even, each nonzero eigenvalue will be evenly degenerate.*

Let $\{\phi_1, \ldots, \phi_{N+2}\}$ *be the set of orthonormal eigenvectors of* γ_Ψ *corresponding to nonzero eigenvalues* $\lambda_1, \ldots, \lambda_{N+2}$*, respectively. Then* Ψ *is a linear combination of, at most,* $\frac{N+1}{2}$ *(*N *odd) or* $\frac{N}{2} + 1$ *(*N *even) Slater determinants constructed from these eigenvectors.*

Proof. If $N = 1$, $\operatorname{rank} \gamma_\Psi$ cannot $N + 2$ by theorem 9. If $N = 2$, in the decomposition 2, $\Psi_a =: \phi_2 \in \mathcal{H}$ is a function of a single particle. Using lemma 13,

$$\gamma_\Psi = \lambda_1 \left| \phi_1 \right\rangle \left\langle \phi_1 \right| + \lambda_1 \left| \phi_2 \right\rangle \left\langle \phi_2 \right| + (1 - \lambda_1)\, \gamma_{\Psi_b},$$

and thus $\lambda_1 < 1$ is at least doubly degenerate. Since $\operatorname{rank} \gamma_{\Psi_b}$ must be equal to 2, Ψ_b is a Slater determinant: $\Psi_b = \phi_3 \wedge \phi_4$ with orthonormal $\phi_1, \ldots, \phi_4$. Finally,

$$\Psi = \sqrt{\lambda_1} \cdot \phi_1 \wedge \phi_2 + \sqrt{1 - \lambda_1} \cdot \phi_3 \wedge \phi_4$$

is a linear combination of 2 Slater determinants, as required. For general N, consider again the decomposition (2):

$$\gamma_\Psi = \lambda_1 \left| \phi_1 \right\rangle \left\langle \phi_1 \right| + \lambda_1 \gamma_{\Psi_a} + (1 - \lambda_1)\, \gamma_{\Psi_b}.$$

The case $\lambda_1 = 1$: then the last term vanishes, and since $a_{\phi_1} \Psi_a = 0$, every eigenvector of γ_{Ψ_a} is also an eigenvector of γ_Ψ with the same eigenvalue. From rank $\gamma_{\Psi_a} = N+1$ we gain the assertion by induction. Note that $\Psi = a^\dagger_{\phi_1}\Psi_a$, hence the number of Slater determinants in the expansion of Ψ and Ψ_a is the same.

The case $\lambda_1 < 1$: we have rank $\gamma_{\Psi_b} \le N+1$ as rank $\gamma_\Psi \ge 1 + \text{rank}\,\gamma_{\Psi_b}$. (Note that γ_{Ψ_a} and γ_{Ψ_b} are positive semidefinite.) By theorem 9, rank $\gamma_{\Psi_b} \neq N+1$, hence rank $\gamma_{\Psi_b} = N$ and Ψ_b is a Slater determinant. Thus, there are orthonormal $\psi_1, \dots, \psi_N \in \mathcal{H}$ such that $\Psi_b = \psi_1 \wedge \cdots \wedge \psi_N$, and γ_{Ψ_b} is an orthogonal projection on the subspace spanned by $\psi_1, \dots, \psi_N$.

We show next that, on the contrary, Ψ_a cannot be a Slater determinant: assuming $\Psi_a = \chi_2 \wedge \cdots \wedge \chi_N$, each χ_i is an eigenvector of γ_{Ψ_a} with eigenvalue 1; thus by lemma 13, it is also an eigenvector of γ_Ψ, and $\langle \chi_i \,|\, \psi_j \rangle = 0$ for all i, j. This means that rank $\gamma_\Psi = 2N$, contradicting the assumptions if $N \ge 3$.

In the sole remaining case rank $\gamma_{\Psi_a} = N+1$, the range of γ_{Ψ_a} must be spanned by $\psi_1, \dots, \psi_N$ and one more additional vector, denoted ψ_{N+1}. Hence Ψ_a can be written as

$$\Psi_a = \sum_{1 \le i_1 < \cdots < i_{N-1} \le N+1} x_{i_1,\dots,i_{N-1}} \cdot \psi_{i_1} \wedge \cdots \wedge \psi_{i_{N-1}}.$$

By 2, for all $i = 1 \dots N$, $x_{1,\dots,i-1,i+1,\dots,N} = \langle \Psi_a \,|\, a_{\psi_i}\Psi_b \rangle = 0$, i.e. only configurations with $i_{N-1} = N+1$ contribute to the sum. Thus ψ_{N+1} is an eigenvector of γ_{Ψ_a} with eigenvalue 1, and - by lemma 13 - also an eigenvector of γ_Ψ. Without loss of generality we may assume $\phi_2 = \psi_{N+1}$.

Applying the decomposition 2 to Ψ_a yields

$$\gamma_{\Psi_a} = |\phi_2\rangle \langle \phi_2| + \gamma_\Phi,$$

where $\Phi \in \wedge^{N-2}\mathcal{H}$ and rank $\gamma_\Phi = N$. Let $\chi_1, \dots, \chi_N$ be the normalized eigenvectors of γ_Φ belonging to nonzero eigenvalues $\mu_1, \dots, \mu_N$, respectively. Since these eigenvectors span the same subspace as $\{\psi_1, \dots, \psi_N\}$, we have $\gamma_{\Psi_b} = \sum_{i=1}^N |\chi_i\rangle \langle \chi_i|$, and without loss of generality, $\Psi_b = \chi_1 \wedge \cdots \wedge \chi_N$.

Putting everything together, it follows that

$$\gamma_\Psi = \lambda_1 |\phi_1\rangle \langle \phi_1| + \lambda_1 |\phi_2\rangle \langle \phi_2| + \sum_{i=1}^N (\lambda_1\mu_i + 1 - \lambda_1) |\chi_i\rangle \langle \chi_i|.$$

Thus we have identified the χ_i's as eigenvectors of γ_Ψ, that is, without loss of generality, $\phi_{i+2} = \chi_i$ for all $i = 1 \dots N$. N cannot be odd, since otherwise, by induction, $\mu_1 = 1$ and ϕ_3 was an eigenvector of γ_Ψ with eigenvalue 1, contradicting $\lambda_1 < 1$. But N being even, each μ_i is evenly degenerate and hence also the eigenvalues of γ_Ψ. Note that

$$\Psi = a^\dagger_{\phi_1}\Psi_a + \Psi_b = a^\dagger_{\phi_1}\Psi_a + \Psi_b = a^\dagger_{\phi_1}a^\dagger_{\phi_2}\Phi + \phi_3 \wedge \cdots \wedge \phi_{N+2}.$$

Since the eigenvectors $\chi_1, \ldots, \chi_N$ of γ_Φ are also eigenvectors of γ_Ψ, the asserted expansion of Ψ follows by induction. $\square$

A generalization of the assertion for the case $N = 2$ in proposition 14 can be found in [4]:

Proposition 15. *Let* $\Psi \in \wedge^N \mathcal{H}$, $\|\Psi\| = 1$. *If* $N \equiv 2 \mod 4$, *then each nonzero eigenvalue of* $\gamma_\Psi^{N/2}$ *is evenly degenerate.*

The proof uses the self-duality of $\gamma_\Psi^{N/2}$.

3.3 Convex Hull of One-Body Density Matrices

It is a well known fact in physics that the ground states of non-interacting many particle systems are Slater determinants. In this section we present a rigorous mathematical proof that Slater determinants actually are the extreme points of the set of one-body density matrices.

Let $\mathcal{H}$ be a separable Hilbert space. For every $A : \mathcal{H} \to \mathcal{H}$ trace class with

$$A\phi = \sum_{i=1}^{\infty} \lambda_i \langle \phi_i \,|\, \phi \rangle \phi_i \quad \forall \phi \in \mathcal{H}, \quad \langle \phi_i \,|\, \phi_j \rangle = \delta_{ij}, \quad \lambda_i \in \mathbb{R},$$

the trace norm equals

$$\|A\|_{\text{trace}} = \sum_{i=1}^{\infty} |\lambda_i| \,. \tag{3}$$

Theorem 16. *Given a separable Hilbert space* $\mathcal{H}$,

$$\begin{aligned}&\overline{\operatorname{conv}\left\{\gamma_\Psi \,|\, \Psi \in \wedge^N \mathcal{H}, \|\Psi\| = 1\right\}}^{\|\cdot\|_{\text{trace}}}\\ &\quad = \left\{g : \mathcal{H} \to \mathcal{H} \,|\, g \text{ selfadjoint}, \, 0 \le g \le 1, \, \operatorname{trace} g = N\right\}.\end{aligned}$$

Designate the left set by L and the right set by R. Note that every $g \in R$ is trace class and hence compact.

Proof.

- "$\subseteq$" follows from $\gamma_\Psi \in R$ for all Ψ as well as R convex and closed with respect to $\|\cdot\|_{\text{trace}}$ since $\|A\| \le \|A\|_{\text{trace}}$ for all $A : \mathcal{H} \to \mathcal{H}$ trace class.

- "$\supseteq$" According to the Hilbert-Schmidt theory for compact self-adjoint operators, every $g \in R$ has a complete orthonormal system $(\phi_i)_{i\in\mathbb{N}}$ of eigenvectors with corresponding eigenvalues $\lambda_i \in \mathbb{R}$, i.e.

$$g\phi = \sum_{i=1}^{\infty} \lambda_i \langle \phi_i \,|\, \phi \rangle \, \phi_i \quad \forall \phi \in \mathcal{H}.$$

We have $0 \le \lambda_i \le 1$ and $\sum_i \lambda_i = \operatorname{trace} g = N$. If $\Psi = \phi_{i_1} \wedge \cdots \wedge \phi_{i_N}$ is a Slater determinant, then

$$\gamma_\Psi \phi = \sum_{k=1}^{N} \langle \phi_{i_k} \,|\, \phi \rangle \, \phi_{i_k} \quad \forall \phi \in \mathcal{H}.$$

The assertion follows now from (3) and the following lemma.

□

Remember that

$$\ell^1 := \left\{ (t_n) \,|\, t_n \in \mathbb{R} \; \forall n \in \mathbb{N}, \sum_{n=1}^{\infty} |t_n| < \infty \right\}$$

is a Banach space over $\mathbb{R}$ with the norm

$$\|t\|_1 := \sum_{n=1}^{\infty} |t_n| \,.$$

Lemma 17. *Let*

$$T := \left\{ t \in \ell^1 \,|\, 0 \le t_n \le 1 \; \forall n, \|t\|_1 = N \right\} \subset \ell^1,$$

then the extreme points are

$$\operatorname{ex} T = \{ t \in T \,|\, t_n \in \{0,1\} \; \forall n \}$$

and

$$T = \overline{\operatorname{conv} \operatorname{ex} T}.$$

Proof. Let $t \in T$ and $0 < t_i < 1$ for an $i \in \mathbb{N}$. Since $\|t\|_1 = N \in \mathbb{N}$, there is an $j \neq i$ such that $0 < t_j < 1$. For $\epsilon > 0$ small enough,

$$r := (t_1, t_2, \dots, t_i + \epsilon, \dots, t_j - \epsilon, \dots) \in T \quad \text{and}$$
$$s := (t_1, t_2, \dots, t_i - \epsilon, \dots, t_j + \epsilon, \dots) \in T.$$

As $t = \frac{1}{2}(r+s)$, $t \notin \operatorname{ex} T$.

Now let $t \in T$, $t_n \in \{0,1\}$ $\forall n$. From $t = \frac{1}{2}(x+y)$ with $x, y \in T$ it follows that $x = y = t$, i.e. $t \in \operatorname{ex} T$.

We show next, by induction with respect to m, that

$$t \in \operatorname{conv} \operatorname{ex} T \quad \forall\, t \in T \text{ with } t_n = 0\ \forall n > m, \quad m \in \mathbb{N} \text{ fixed.}$$

$m = N$: then $t \in \operatorname{ex} T$.
$m = N+1$: set

$$s_n^i := \begin{cases} 1 & n \neq i, 1 \leq n \leq N+1 \\ 0 & \text{otherwise} \end{cases}, \quad i = 1, \ldots, N+1.$$

Then $s^i \in \operatorname{ex} T$ and $t = \sum_{i=1}^{N+1} (1 - t_i)\, s^i$.
$m > N+1$: without loss of generality $t_m \neq 0$ and $t_n \geq t_m$ $\forall n = 1, \ldots, m$. Set

$$s_n := \begin{cases} 1 & m - N < n \leq m \\ 0 & \text{otherwise} \end{cases}$$

and

$$r := \frac{1}{1 - t_m}\,[t - t_m s] \in T.$$

By induction, $r \in \operatorname{conv} \operatorname{ex} T$, hence also

$$t = (1 - t_m) r + t_m s \in \operatorname{conv} \operatorname{ex} T.$$

Finally, let $t \in T$. Given $\epsilon > 0$, choose $m \in \mathbb{N}$ with $\sum_{n>m} |t_n| < \frac{\epsilon}{2}$. Without loss of generality $t_m \leq 1 - \frac{\epsilon}{2}$. Set

$$r_n := \begin{cases} t_n & n < m \\ t_m + \sum_{k>m} t_k & n = m \\ 0 & n > m \end{cases},$$

then $r \in \operatorname{conv} \operatorname{ex} T$ by the above result and $\|t - r\|_1 < \epsilon$. □

4 Conjectures and Further Ideas

In the previous section we have focused on the one-body density matrix γ_Ψ. Although our goal is the two-body matrix, this is useful since we might gain - as already mentioned - a simplification scheme.

More specifically, if for example $\dim \mathcal{H} = 6$ and $N = 4$, by proposition 14, we will require 3 instead of $\binom{6}{4} = 15$ coefficients (denoted α, β, γ) to represent Ψ. An explicit calculation shows that the entries of the matrix representation of Γ_Ψ have the form $|\alpha|^2, \overline{\alpha}\beta, |\alpha|^2+|\beta|^2$, so a concrete calculation of the convex hull lies at hand.

By the unitary freedom stated in proposition 10, we may without loss of generality assume that γ_Ψ is diagonal, by using the eigenvectors of γ_Ψ as basis.

The decomposition scheme for γ_Ψ might be applied to Γ_Ψ as well.

Numerical experiments give rise to the following conjectures:

- For general p, γ_Ψ^p is an orthogonal projection iff Ψ is a Slater determinant.
- $\max_\Psi \|\gamma_\Psi^p\|_{\text{fro}}$ is reached iff γ_Ψ^p is an orthonormal projection (i.e. the maximum is $\binom{N}{p}$)).

5 Conclusion

In this thesis we have provided a firm ground for the further investigation of reduced density matrices. A good comprehension of the one-body matrix promises to be useful in the two-body case. Proposition 14 shows that, in the case $\operatorname{rank}\gamma_\Psi = N+2$, the wave function is composed of an order N (instead of N^2) Slater determinants, and that these are constructed from the eigenvectors of the one-body density matrix. Recent progress for $N = 4$ [1] suggests that further studies are promising and new insights can be gained.

6 Appendix

6.1 Basic Properties of Integral Operators

Theorem 18. *Let $(\Omega, \mathcal{A}, \mu)$ be a σ-finite measure space and $\gamma \in L^2(\Omega\times\Omega, \mathbb{C})$ such that $\gamma(x,y) = \overline{\gamma(y,x)}$ $\forall x, y \in \Omega$. Then*

$$\Gamma: \ L^2(\Omega,\mathbb{C}) \to L^2(\Omega,\mathbb{C}), \ (\Gamma\phi)(x) := \int \gamma(x,y)\phi(y)\,\mathrm{d}y$$

is linear, compact and self-adjoint.

Proof. Γ is well-defined: by a theorem of measure and integration theory,

$$\gamma_x: \ y \mapsto \overline{\gamma(x,y)} \ \in L^2(\Omega,\mathbb{C})$$

for almost all $x \in \Omega$. Using the inner product of $L^2(\Omega,\mathbb{C})$, we may write

$$(\Gamma\phi)(x) = \langle \gamma_x \,|\, \phi \rangle \,.$$

Thus

$$\int |(\Gamma\phi)(x)|^2 \, \mathrm{d}x \leq \int \|\gamma_x\|^2 \|\phi\|^2 \, \mathrm{d}x = \left(\int\int |\gamma(x,y)|^2 \, \mathrm{d}y \, \mathrm{d}x\right) \|\phi\|^2 < \infty.$$

Γ is compact: let $(\phi_i)_{i\in\mathbb{N}}$ be a bounded sequence in $L^2(\Omega,\mathbb{C})$. Then there exists a weakly convergent subsequence (also denoted by (ϕ_i)), i.e. $\phi_i \rightharpoonup \phi \in L^2(\Omega,\mathbb{C})$. Therefore

$$(\Gamma\phi_i)(x) = \langle \gamma_x \,|\, \phi_i \rangle \to \langle \gamma_x \,|\, \phi \rangle = (\Gamma\phi)(x) \quad \text{for almost all } x \in \Omega.$$

Choose $M \in \mathbb{R}$ such that $\|\phi_i\| \leq M$ for all $i \in \mathbb{N}$, then

$$|(\Gamma\phi_i)(x)| = |\langle \gamma_x \,|\, \phi_i \rangle| \leq M \cdot \|\gamma_x\| \in L^2(\Omega,\mathbb{C}).$$

The theorem of dominated convergence now yields $\Gamma\phi_i \xrightarrow{L^2} \Gamma\phi$.

Γ is self-adjoint: for all $\phi,\psi \in L^2(\Omega,\mathbb{C})$ we have

$$\langle \psi \,|\, \Gamma\phi \rangle = \int\int \overline{\psi(x)}\gamma(x,y)\phi(y) \, \mathrm{d}y \, \mathrm{d}x = \int\int \overline{\gamma(y,x)\psi(x)}\phi(y) \, \mathrm{d}x \, \mathrm{d}y = \langle \Gamma\psi \,|\, \phi \rangle .$$

□

Now, let further $L^2(\Omega,\mathbb{C})$ be separable, e.g. $(\Omega,\mathcal{A},\mu) = (\mathbb{R}^N,\mathcal{B},\lambda)$.

Proposition 19. *Let Γ be positive semidefinite. Then*

$$\operatorname{trace}\Gamma = \int \gamma(x,x) \, \mathrm{d}x \in [0,\infty].$$

Proof. By the spectral theorem for compact, self-adjoint operators, Γ has a complete orthonormal system $(\psi_i)_{i\in\mathbb{N}}$ of eigenvectors with corresponding eigenvalues $\lambda_i \in \mathbb{R}$. That is,

$$\Gamma\phi = \sum_i \lambda_i \langle \psi_i \,|\, \phi \rangle \, \psi_i \quad \forall\phi \in L^2(\Omega,\mathbb{C}), \quad \text{and}$$

$$\gamma_x = \sum_i \langle \psi_i \,|\, \gamma_x \rangle \, \psi_i = \sum_i \overline{(\Gamma\psi_i)(x)} \, \psi_i = \sum_i \lambda_i \, \overline{\psi_i(x)} \, \psi_i, \quad \text{i.e.}$$

$$\gamma(x,y) = \overline{\gamma_x(y)} = \sum_i \lambda_i \, \psi_i(x) \, \overline{\psi_i(y)}.$$

As Γ is positive semidefinite, $\lambda_i \geq 0 \; \forall i \in \mathbb{N}$; thus the theorem of monotone convergence yields

$$\operatorname{trace}\Gamma = \sum_i \lambda_i = \int \sum_i \lambda_i \, |\psi_i(x)|^2 \, \mathrm{d}x = \int \gamma(x,x) \, \mathrm{d}x.$$

□

6.2 The Tensor Product of Hilbert Spaces

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces over $\mathbb{K} = \mathbb{R}$ or $\mathbb{C}$ and $u \in \mathcal{H}_1$, $v \in \mathcal{H}_2$. Define

$$(u \otimes v)(w, z) := \langle w \,|\, u \rangle \langle z \,|\, v \rangle \quad \text{for all } w \in \mathcal{H}_1,\ z \in \mathcal{H}_2.$$

$u \otimes v$ is a conjugate bilinear form on $\mathcal{H}_1 \times \mathcal{H}_2$. Note that $u \otimes v$ equals $u' \otimes v'$ iff the corresponding forms are identical and that $\otimes$ behaves like a product, i.e.

$$(\alpha u + u') \otimes v = \alpha (u \otimes v) + (u' \otimes v), \quad \alpha \in \mathbb{K}$$

and similarly for $u \otimes (\alpha v + v')$. Denote the set of all finite linear combinations of such forms by $(\mathcal{H}_1 \otimes \mathcal{H}_2)_{\text{pre}}$. This becomes a pre-Hilbert space with the inner product

$$\langle u \otimes v \,|\, w \otimes z \rangle := \langle u \,|\, w \rangle \langle v \,|\, z \rangle = (w \otimes z)(u, v),$$

extending linearly. To show that this definition doesn't depend on the choice of representatives, first let μ be a finite linear combination which is the zero form. Then

$$\langle u \otimes v \,|\, \mu \rangle = \mu(u, v) = 0 \quad \text{for all } u \in \mathcal{H}_1,\ v \in \mathcal{H}_2$$

and by linearity $\langle \lambda \,|\, \mu \rangle = 0$ for all $\lambda \in (\mathcal{H}_1 \otimes \mathcal{H}_2)_{\text{pre}}$. Given finite sums $\lambda, \lambda', \mu, \mu'$ with $\lambda = \lambda'$ and $\mu = \mu'$, we now have

$$\langle \lambda \,|\, \mu \rangle - \langle \lambda' \,|\, \mu' \rangle = \langle \lambda \,|\, \mu - \mu' \rangle + \overline{\langle \mu' \,|\, \lambda - \lambda' \rangle} = 0.$$

Finally, we show that the inner product is positive definite. Suppose

$$\lambda = \sum_{i=1}^{N} \alpha_i (u_i \otimes v_i), \quad u_i \in \mathcal{H}_1,\ v_i \in \mathcal{H}_2.$$

Let $(w_i)_i$ and $(z_i)_i$ be finite orthonormal bases of $\operatorname{span}\{u_i\}_{i=1\ldots N}$ and $\operatorname{span}\{v_i\}_{i=1\ldots N}$, respectively. Expressing each u_i in terms of the w_i's and each v_i in terms of the z_i's, we obtain

$$\lambda = \sum_{i,j} \beta_{ij} (w_i \otimes z_j).$$

Thus

$$\langle \lambda \,|\, \lambda \rangle = \sum_{i,j,k,m} \overline{\beta_{ij}} \beta_{km} \langle w_i \,|\, w_k \rangle \langle z_j \,|\, z_m \rangle = \sum_{i,j} |\beta_{ij}|^2 \geq 0,$$

and $\langle \lambda \,|\, \lambda \rangle = 0$ iff $\lambda = 0$.

Definition 20. *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces over $\mathbb{K}$. The* tensor product *$\mathcal{H}_1 \otimes \mathcal{H}_2$ is the completion of $(\mathcal{H}_1 \otimes \mathcal{H}_2)_{pre}$.*

Theorem 21. *If $(u_i)_{i\in\mathbb{N}}$ and $(v_i)_{i\in\mathbb{N}}$ are complete orthonormal systems in the Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively, then $(u_i \otimes v_j)_{i,j\in\mathbb{N}}$ is a complete orthonormal system in $\mathcal{H}_1 \otimes \mathcal{H}_2$.*

Proof. $(u_i \otimes v_j)_{i,j\in\mathbb{N}}$ is orthonormal, so what remains to be shown is completeness, i.e. $\operatorname{span}(u_i \otimes v_j)_{i,j\in\mathbb{N}}$ is dense in $\mathcal{H}_1 \otimes \mathcal{H}_2$. It is sufficient to proof that $(\mathcal{H}_1 \otimes \mathcal{H}_2)_{\text{pre}}$ is contained in the closure of this span. Let $u \in \mathcal{H}_1$, $v \in \mathcal{H}_2$. We have

$$u = \sum_{i=1}^{\infty} \underbrace{\langle u_i \,|\, u \rangle}_{\alpha_i} u_i, \quad v = \sum_{i=1}^{\infty} \underbrace{\langle v_i \,|\, v \rangle}_{\beta_i} v_i.$$

Since $\sum_{i,j} |\alpha_i\beta_j|^2 = \sum_i |\alpha_i|^2 \sum_j |\beta_j|^2 < \infty$, the infinite series

$$\lambda := \lim_{N\to\infty} \sum_{i,j=1}^{N} \alpha_i\beta_j \,(u_i \otimes v_j)$$

converges in $\mathcal{H}_1 \otimes \mathcal{H}_2$, and

$$\left\| (u \otimes v) - \sum_{i,j=1}^{N} \alpha_i\beta_j \,(u_i \otimes v_j) \right\|^2 = \|u\|^2 \|v\|^2 - \sum_{i,j=1}^{N} |\alpha_i\beta_j|^2 \to 0.$$

□

We want to rigorously justify the "natural" isomorphism between L^2-spaces as follows.

Theorem 22. *Given two σ-finite measure spaces $(\Omega_1, \mathcal{A}_1, \mu_1)$, $(\Omega_2, \mathcal{A}_2, \mu_2)$ and assuming that the Hilbert spaces $L^2(\Omega_1, \mu_1)$ and $L^2(\Omega_2, \mu_2)$ are separable, there exists an isomorphism*

$$U : L^2(\Omega_1, \mu_1) \otimes L^2(\Omega_2, \mu_2) \to L^2(\Omega_1 \times \Omega_2, \mu_1 \otimes \mu_2)$$

so that

$$(Uf \otimes g)\,(x, y) = f(x)g(y) \quad \text{for all } f \in L^2(\Omega_1, \mu_1),\ g \in L^2(\Omega_2, \mu_2). \tag{4}$$

Proof. Let $(\phi_i)_{i\in\mathbb{N}}$ and $(\psi_i)_{i\in\mathbb{N}}$ be complete orthonormal systems in $L^2(\Omega_1,\mu_1)$ and $L^2(\Omega_2,\mu_2)$, respectively. Then $(\phi_i(x)\psi_j(y))_{i,j\in\mathbb{N}}$ is a complete orthonormal system in $L^2(\Omega_1\times\Omega_2,\mu_1\otimes\mu_2)$. The orthonormality is obvious, and the completeness can be seen as follows: let $h\in L^2(\Omega_1\times\Omega_2,\mu_1\otimes\mu_2)$ and suppose that for all i,j

$$\int_{\Omega_1\times\Omega_2}\overline{\phi_i(x)\psi_j(y)}h(x,y)\,\mathrm{d}x\,\mathrm{d}y=0,$$

i.e.

$$\int_{\Omega_1}\overline{\phi_i(x)}\left(\int_{\Omega_2}\overline{\psi_j(y)}h(x,y)\,\mathrm{d}y\right)\,\mathrm{d}x=0.$$

Since $(\phi_i)_i$ is complete, this means that up to a set of measure zero, the inner integral is zero for all $x\in\Omega_1$. Since $(\psi_i)_i$ is also complete, $h(x,y)=0$ almost everywhere.

Now define U by

$$(U\phi_i\otimes\phi_j)(x,y):=\phi_i(x)\psi_j(y).$$

U is a mapping between orthonormal systems and hence unitary. Note that we recover equation (4). □

The tensor product

$$\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_n$$

of finitely many Hilbert spaces is a canonical extension of the above definitions.

In quantum mechanics, the Pauli exclusion principle states that multiple identical Fermions may not occupy the same state simultaneously. This translates to the antisymmetrization of wave functions.

Standard Example 23. *Let $(u_i)_{i\in\mathbb{N}}$ be a complete orthonormal system in the Hilbert space $\mathcal{H}$. For each permutation $\sigma\in S_n$, define an unitary operator given on basis elements of $\otimes^n\mathcal{H}$ by*

$$\sigma\left(u_{i_1}\otimes\cdots\otimes u_{i_n}\right):=u_{i_{\sigma(1)}}\otimes\cdots\otimes u_{i_{\sigma(n)}}.$$

The n-fold antisymmetric tensor product $\wedge^n\mathcal{H}$ *of $\mathcal{H}$ is the image of the orthogonal projection*

$$A_n:=\frac{1}{n!}\sum_{\sigma\in S_n}sgn(\sigma)\sigma.$$

Note that $\wedge^n\mathcal{H}$ is itself a Hilbert space. Set

$$u_{i_1}\wedge\cdots\wedge u_{i_n}:=\sqrt{n!}\,A_n\left(u_{i_1}\otimes\cdots\otimes u_{i_n}\right),$$

then $(u_{i_1} \wedge \cdots \wedge u_{i_n})_{i_1 < i_2 < \cdots < i_n}$ *is a complete orthonormal system in* $\wedge^n \mathcal{H}$*. In the special case where* $\mathcal{H} = L^2(\Omega, \mu)$ *and* $(\Omega, \mathcal{A}, \mu)$ *is* σ*-finite,* $\wedge^n \mathcal{H}$ *is the set of all antisymmetric* L^2*-functions, i.e.*

$$\wedge^n \mathcal{H} \simeq L^2(\Omega^n, \otimes^n \mu)_{anti} := \\ \big\{ \phi \in L^2(\Omega^n, \otimes^n \mu) \;|\, \phi(\ldots, x_i, \ldots, x_j, \ldots) \\ = -\phi(\ldots, x_j, \ldots, x_i, \ldots) \;\forall i \neq j \;\big\}$$

It is obvious that σ is unitary as it permutes the orthonormal system $(u_{i_1} \otimes \cdots \otimes u_{i_n})_{i_1, \ldots i_n \in \mathbb{N}}$. We show that σ is independent of the choice of $(u_i)_i$. Let $v_1, \ldots, v_n \in \mathcal{H}$ and set $\alpha_{ij} := \langle u_i \,|\, v_j \rangle$. Then

$$\langle u_{i_1} \otimes \cdots \otimes u_{i_n} \,|\, v_1 \otimes \cdots \otimes v_n \rangle = \alpha_{i_1 1} \cdots \alpha_{i_n n}$$

and hence

$$\begin{aligned} \sigma\left(v_1 \otimes \cdots \otimes v_n\right) &= \sum_{i_1, \ldots, i_n} \alpha_{i_1 1} \cdots \alpha_{i_n n} \cdot u_{i_{\sigma(1)}} \otimes \cdots \otimes u_{i_{\sigma(n)}} \\ &= \sum_{i_1, \ldots, i_n} \alpha_{i_1 \sigma(1)} \cdots \alpha_{i_n \sigma(n)} \cdot u_{i_1} \otimes \cdots \otimes u_{i_2} \\ &= v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(n)}. \end{aligned}$$

It is easy to see that A_n is a linear, continuous, self-adjoint operator, and from $\sigma A_n = \operatorname{sgn}(\sigma) A_n$ we get $A_n^2 = A_n$, so A_n is an orthogonal projection. Note that

$$\operatorname{span}\{A_n\left(u_{i_1} \otimes \cdots \otimes u_{i_n}\right)\}_{i_1, \ldots, i_n \in \mathbb{N}}$$

is dense in $\wedge^n \mathcal{H}$ and $(A_n \sigma)\left(u_{i_1} \otimes \cdots \otimes u_{i_n}\right) = \operatorname{sgn}(\sigma) A_n\left(u_{i_1} \otimes \cdots \otimes u_{i_n}\right)$. We remark that for another orthonormal system $(v_i)_{i \in \mathbb{N}}$, the inner product has a special form:

$$\begin{aligned} &\langle v_1 \wedge \cdots \wedge v_n \,|\, u_1 \wedge \cdots \wedge u_n \rangle \\ &= n! \,\langle v_1 \otimes \cdots \otimes v_n \,|\, A_n(u_1 \otimes \cdots \otimes u_n) \rangle \\ &= \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) \prod_{\alpha=1}^{n} \left\langle v_\alpha \,|\, u_{\sigma(\alpha)} \right\rangle = \det \left\langle v_\alpha \,|\, u_\beta \right\rangle_{\alpha, \beta}. \end{aligned}$$

If $\mathcal{H} = L^2(\Omega, \mu)$, theorem 22 states

$$\otimes^n \mathcal{H} \simeq L^2(\Omega^n, \otimes^n \mu);$$

for each $\phi \in L^2(\Omega^n, \otimes^n \mu)$, a basis expansion shows that

$$(A_n\phi)(x_1, \ldots, x_n) = \frac{1}{n!} \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) \phi\left(x_{\sigma(1)}, \ldots, x_{\sigma(n)}\right),$$

so $A_n\phi$ is antisymmetric. Conversely, if ϕ is antisymmetric, then it's left invariant by A_n.

Proposition 24. *Let $(u_i)_{i\in\mathbb{N}}$ be a complete orthonormal system in the Hilbert space $\mathcal{H}$ and $U : \mathcal{H} \to \mathcal{H}$ an unitary operator. Then the operator (again denoted by U) given on basis elements of $\otimes^n\mathcal{H}$ by*

$$U(u_{i_1} \otimes \cdots \otimes u_{i_n}) := (Uu_{i_1}) \otimes \cdots \otimes (Uu_{i_n})$$

is unitary and leaves $\wedge^n\mathcal{H}$ invariant.

Proof. It follows directly from the definitions that $U : \operatorname{span}\{u_{i_1} \otimes \cdots \otimes u_{i_n}\}_{i_1,\ldots,i_n} \to \operatorname{span}\{Uu_{i_1} \otimes \cdots \otimes Uu_{i_n}\}_{i_1,\ldots,i_n}$ is bijective and preserves norms. That is, U extends uniquely to an unitary operator $U : \otimes^n\mathcal{H} \to \otimes^n\mathcal{H}$. Furthermore $A_nU = UA_n$ as

$$\begin{aligned} &A_nU(u_{i_1} \otimes \cdots \otimes u_{i_n}) \\ &= \frac{1}{n!} \sum_{\sigma \in S_n} \operatorname{sgn}(\sigma) Uu_{i_{\sigma(1)}} \otimes \cdots \otimes Uu_{i_{\sigma(n)}} \\ &= UA_n(u_{i_1} \otimes \cdots \otimes u_{i_n}). \end{aligned}$$

From that it follows that the restriction U: $\wedge^n\mathcal{H} \to \wedge^n\mathcal{H}$ on the Hilbert space $\wedge^n\mathcal{H}$ is also unitary. □

We investigate vector-valued functions and their connection with tensor products.

Definition 25. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space and $\mathcal{H}'$ a separable Hilbert space. A function $f : \Omega \to \mathcal{H}'$ is called* measurable *iff $x \mapsto \langle y \mid f(x)\rangle$ is measurable for each $y \in \mathcal{H}'$. We set*

$$L^2(\Omega, \mu; \mathcal{H}') := \left\{ f : \Omega \to \mathcal{H}' \mid f \text{ measurable}, \int_\Omega \|f(x)\|^2 \, \mathrm{d}x < \infty \right\}.$$

We have to justify that $\|f(x)\|^2$ is measurable. Let $(u_i)_i$ be a complete orthonormal system in $\mathcal{H}'$. Then by definition, $x \mapsto \langle u_i \mid f(x)\rangle$ is measurable and hence also

$$x \mapsto \|f(x)\|^2 = \sum_i |\langle u_i \mid f(x)\rangle|^2.$$

Note that since an inner product can be expressed by norms, $x \mapsto \langle f(x) \mid g(x)\rangle$ is also measurable for all $f, g \in L^2(\Omega, \mu; \mathcal{H}')$.

Proposition 26. *$L^2(\Omega, \mu; \mathcal{H}')$ given above is a Hilbert space with the inner product*

$$\langle f \,|\, g\rangle := \int_\Omega \langle f(x) \,|\, g(x)\rangle \, \mathrm{d}x.$$

Proof. Most results obtained for $L^2(\Omega, \mu)$ generalize literally to $L^2(\Omega, \mu; \mathcal{H}')$, especially the theorem by F. Riesz and E. Fischer which states the completeness of $L^2(\Omega, \mu)$. In this connection, e.g. note that given a sequence $(u_i)_i$ in $\mathcal{H}'$ with $\sum_{i=1}^\infty \|u_i\| < \infty$, the sequence of partial sums

$$s_n := \sum_{i=1}^n u_i$$

converges in $\mathcal{H}'$ since it is a Cauchy sequence:

$$\|s_{n+k} - s_n\| = \left\| \sum_{i=n+1}^{n+k} u_i \right\| \leq \sum_{i=n+1}^{n+k} \|u_i\| \to 0 \quad \text{as } n \to \infty.$$

Thus we have generalized the well-known classical result on $\mathbb{C}$ that each absolutely convergent series is convergent. □

Theorem 27. *Let $(\Omega, \mathcal{A}, \mu)$ be a measure space such that $L^2(\Omega, \mu)$ is separable and let $\mathcal{H}'$ be a separable Hilbert space. Then there exists an isomorphism*

$$U : L^2(\Omega, \mu) \otimes \mathcal{H}' \to L^2(\Omega, \mu; \mathcal{H}')$$

such that

$$(Uf \otimes u)(x) = f(x)u \quad \textit{for all } f \in L^2(\Omega, \mu),\ u \in \mathcal{H}'.$$

Proof. Choose complete orthonormal systems $(\phi_i)_{i\in\mathbb{N}}$ and $(u_i)_{i\in\mathbb{N}}$ of $L^2(\Omega, \mu)$ and $\mathcal{H}'$, respectively. Obviously, $(\phi_i u_j)_{i,j}$ is orthonormal; we show that it's also complete. Given $f \in L^2(\Omega, \mu; \mathcal{H}')$, let

$$h_j \in L^2(\Omega, \mu), \quad h_j(x) := \langle u_j \,|\, f(x)\rangle$$

and $\alpha_{ij} := \langle \phi_i u_j \,|\, f\rangle = \langle \phi_i \,|\, h_j\rangle$. Then by the theorem of monotone convergence,

$$\begin{aligned}\sum_{i,j} |\alpha_{ij}|^2 &= \sum_j \|h_j\|^2 = \int_\Omega \sum_j |h_j(x)|^2 \, \mathrm{d}x \\ &= \int_\Omega \sum_j |\langle u_j \,|\, f(x)\rangle|^2 \, \mathrm{d}x = \int_\Omega \|f(x)\|^2 \, \mathrm{d}x = \|f\|^2 < \infty\end{aligned}$$

and hence $\sum_{i,j=1}^{\infty} \alpha_{ij}\phi_i u_j$ converges in $L^2(\Omega, \mu; \mathcal{H}')$. Furthermore,

$$\left\| f - \sum_{i,j=1}^{N} \alpha_{ij}\phi_i u_j \right\|^2 = \|f\|^2 - \sum_{i,j=1}^{N} |\alpha_{ij}|^2 \to 0 \quad \text{as } N \to \infty.$$

Now define U by

$$\left(U\phi_i \otimes u_j\right)(x) := \phi_i(x)u_j,$$

which maps an orthonormal system to an orthonormal system and hence extends uniquely to an unitary operator. □

6.3 Second Quantization (Fermions)

6.3.1 Introduction

The common term "Second Quantization" is somewhat misleading as it is just an efficient formalism for many-particle systems. Here we will consider fermions only (spin 1/2 particles). The spin-statistic theorem of relativistic quantum field theory states that fermions must be antisymmetric, i.e. the wave function changes sign under exchange of two identical particles.

6.3.2 Preliminaries

Let $\mathcal{H}$ be a Hilbert space and $\otimes^N\mathcal{H}$ the Hilbert space tensor product. $\wedge^N\mathcal{H}$ is the image of the orhogonal projection defined by

$$A_N\left(\phi_1 \otimes \cdots \otimes \phi_N\right) := \frac{1}{N!}\sum_{\sigma\in S_N} \operatorname{sgn}(\sigma)\phi_{\sigma(1)} \otimes \cdots \otimes \phi_{\sigma(N)}$$

(i.e. A_N is a linear, continuous, self-adjoint operator with $A_N^2 = A_N$). Physically speaking, $\wedge^N\mathcal{H}$ is the space where the antisymmetric many-particle function lives.

By definition, a Slater determinant is of the form

$$\phi_1 \wedge \cdots \wedge \phi_N := \sqrt{N!}\, A_N\left(\phi_1 \otimes \cdots \otimes \phi_N\right),$$

where $\phi_1, \ldots \phi_N \in \mathcal{H}$. If $\langle \phi_\alpha \,|\, \phi_\beta \rangle = \delta_{\alpha\beta}$, then it will be normalized.

Since $A_N^* = A_N$ and $A_N^2 = A_N$, the following holds:

$$\begin{aligned}
&\langle \phi_1 \wedge \cdots \wedge \phi_N \,|\, \psi_1 \wedge \cdots \wedge \psi_N \rangle \\
&= N!\, \langle \phi_1 \otimes \cdots \otimes \phi_N \,|\, A_N(\psi_1 \otimes \cdots \otimes \psi_N) \rangle \\
&= \sum_{\sigma\in S_N} \operatorname{sgn}(\sigma) \prod_{\alpha=1}^{N} \left\langle \phi_\alpha \,|\, \psi_{\sigma(\alpha)} \right\rangle = \det \langle \phi_\alpha \,|\, \psi_\beta \rangle_{\alpha,\beta}\,.
\end{aligned}$$

Remark: Let $(\phi_i)_i$ be a complete orthonormal system of $\mathcal{H}$. Then

$$(\phi_{i_1} \wedge \cdots \wedge \phi_{i_N})_{i_1 < i_2 < \cdots < i_N}$$

is a complete orthonormal system of $\wedge^N \mathcal{H}$.

6.3.3 Creation and Annihilation Operators

Let $(\phi_i)_i$ be a complete orthonormal system in the Hilbert space $\mathcal{H}$. When appropriate, we set $|i\rangle = \phi_i$. Furthermore, let $\phi, \psi \in \mathcal{H}$ and assume that $\psi_1, \ldots, \psi_N \in \mathcal{H}$ are orthonormal. We define a creation operator by

$$a_\phi^\dagger \, \psi_1 \wedge \cdots \wedge \psi_N := \phi \wedge \psi_1 \wedge \cdots \wedge \psi_N,$$

extending linearly. The adjoint "annihilation" operator is then

$$a_\phi \, \psi_1 \wedge \cdots \wedge \psi_N := \sum_{\alpha=1}^{N} (-1)^{\alpha+1} \langle \phi \,|\, \psi_\alpha \rangle \, \psi_1 \wedge \ldots \psi_{\alpha-1} \wedge \psi_{\alpha+1} \cdots \wedge \psi_N.$$

This can be seen from the column expansion theorem for determinants:

$$\begin{aligned}
&\left\langle \psi_1 \wedge \cdots \wedge \psi_N \,\middle|\, a_\phi^\dagger \, \chi_1 \wedge \cdots \wedge \chi_{N-1} \right\rangle \\
&= \sum_{\gamma=1}^{N} (-1)^{\gamma+1} \langle \psi_\gamma \,|\, \phi \rangle \det \langle \psi_\alpha \,|\, \chi_\beta \rangle_{\alpha \neq \gamma, \beta} \\
&= \langle a_\phi \, \psi_1 \wedge \cdots \wedge \psi_N \,|\, \chi_1 \wedge \cdots \wedge \chi_{N-1} \rangle \, .
\end{aligned}$$

From a physical point of view, these operators increase/decrease the particle number by one. We write $a_i^\dagger := a_{\phi_i}^\dagger$ and $a_i := a_{\phi_i}$. The anticommutator brackets yield

$$\{a_\phi, a_\psi\} = 0, \quad \left\{a_\phi^\dagger, a_\psi^\dagger\right\} = 0, \quad \left\{a_\phi, a_\psi^\dagger\right\} = \langle \phi \,|\, \psi \rangle \, .$$

The "occupation number operator" for the state ϕ,

$$\hat{n}_\phi := a_\phi^\dagger a_\phi,$$

derives its name from the following property:

$$\hat{n}_{\phi_j} \phi_{i_1} \wedge \cdots \wedge \phi_{i_N} = \begin{cases} 1 & j \in \{i_1, \ldots, i_N\} \\ 0 & \text{otherwise} \end{cases}$$

Given the operator $T : \mathcal{H} \to \mathcal{H}$, we want to rewrite

$$\tilde{T} = \sum_{\alpha=1}^{N} T_\alpha \qquad (T_\alpha \text{ acting on the } \alpha\text{-th particle})$$

in terms of creation and annihilation operators.

$$\begin{aligned}
&\left(\sum_{\alpha=1}^{N} |\phi\rangle_\alpha \langle\chi|_\alpha\right) \psi_1 \wedge \cdots \wedge \psi_N \\
&= \sum_{\alpha=1}^{N} \langle \chi \,|\, \psi_\alpha \rangle \, (-1)^{\alpha+1} a_\phi^\dagger \; \psi_1 \wedge \ldots \psi_{\alpha-1} \wedge \psi_{\alpha+1} \cdots \wedge \psi_N \\
&= a_\phi^\dagger a_\chi \; \psi_1 \wedge \cdots \wedge \psi_N, \quad \text{i.e.} \\
&\sum_{\alpha=1}^{N} |\phi\rangle_\alpha \langle\chi|_\alpha = a_\phi^\dagger a_\chi,
\end{aligned}$$

so we have

$$\tilde{T} = \sum_{\alpha=1}^{N} \sum_{i,j} \langle i \,|\, T\, j \rangle \, |i\rangle_\alpha \langle j|_\alpha = \sum_{i,j} \langle i \,|\, T\, j\rangle \, a_i^\dagger a_j.$$

In order to handle two-particle interactions, we first define pair creation and annihilation operators by

$$\begin{aligned}
a_{\phi\wedge\psi}^\dagger &:= a_\phi^\dagger a_\psi^\dagger, \qquad \text{extending to} \quad a^\dagger_{\phi_1\wedge\psi_1 + c\,\phi_2\wedge\psi_2} = a^\dagger_{\phi_1\wedge\psi_1} + c\, a^\dagger_{\phi_2\wedge\psi_2} \\
a_{\phi\wedge\psi} &:= \left(a_{\phi\wedge\psi}^\dagger\right)^* = a_\psi a_\phi.
\end{aligned}$$

Now use $\delta_{kj} = \left\{a_k, a_j^\dagger\right\}$ to get

$$\begin{aligned}
\sum_{\alpha\neq\beta} |i\rangle_\alpha |j\rangle_\beta \langle k|_\alpha \langle l|_\beta &= \sum_{\alpha\neq\beta} |i\rangle_\alpha \langle k|_\alpha |j\rangle_\beta \langle l|_\beta \\
&= \sum_{\alpha,\beta} |i\rangle_\alpha \langle k|_\alpha |j\rangle_\beta \langle l|_\beta - \delta_{kj} \sum_\alpha |i\rangle_\alpha \langle l|_\alpha \\
&= a_i^\dagger a_k a_j^\dagger a_l - a_i^\dagger \left\{a_k, a_j^\dagger\right\} a_l = -a_i^\dagger a_j^\dagger a_k a_l \\
&= a_{i\wedge j}^\dagger a_{k\wedge l}.
\end{aligned}$$

Given a pair operator V, applying the above result yields

$$\begin{aligned}
\tilde{V} &:= \frac{1}{2}\sum_{\alpha\neq\beta} V_{\alpha,\beta} \\
&= \frac{1}{2}\sum_{\alpha\neq\beta}\sum_{i,j,k,l} \langle i\otimes j\,|\,V\; k\otimes l\rangle\, |i\rangle_\alpha\, |j\rangle_\beta\, \langle k|_\alpha\, \langle l|_\beta \\
&= \frac{1}{2}\sum_{i,j,k,l} \langle i\otimes j\,|\,V\; k\otimes l\rangle\, a^\dagger_{i\wedge j} a_{k\wedge l} \\
&= \frac{1}{2}\sum_{i<j,\,k<l} \langle i\otimes j - j\otimes i\,|\,V\; (k\otimes l - l\otimes k)\rangle\, a^\dagger_{i\wedge j} a_{k\wedge l} \\
&= \sum_{i<j,\,k<l} \langle i\wedge j\,|\,V\; k\wedge l\rangle\, a^\dagger_{i\wedge j} a_{k\wedge l},
\end{aligned}$$

that is, given a complete orthonormal system $(\chi_i)_i$ in $\wedge^2\mathcal{H}$,

$$\tilde{V} = \sum_{i,j} \langle \chi_i\,|\,V\chi_j\rangle\, a^\dagger_{\chi_i} a_{\chi_j}.$$

Let's investigate the special case

$$V = |\chi\rangle\langle\chi|, \quad \chi\in\wedge^2\mathcal{H}:$$

$$\tilde{V} = \sum_i \langle\chi_i\,|\,\chi\rangle\, a^\dagger_{\chi_i} \sum_j \langle\chi\,|\,\chi_j\rangle\, a_{\chi_j} = a^\dagger_\chi a_\chi \equiv \hat{n}_\chi.$$

Note that the pair operators have bosonic character. A short computation shows that

$$\left[a^\dagger_{i\wedge j}, a^\dagger_{k\wedge l}\right] = 0,$$

and, taking the adjoints,

$$[a_{i\wedge j}, a_{k\wedge l}] = 0.$$

Using

$$\left[a_i, a^\dagger_k a^\dagger_l\right] = a_i a^\dagger_k a^\dagger_l - a^\dagger_k a^\dagger_l a_i = \delta_{ik} a^\dagger_l - \delta_{il} a^\dagger_k,$$

we get

$$\left[a_{i\wedge j}, a^\dagger_{k\wedge l}\right] = \left[a_j a_i, a^\dagger_k a^\dagger_l\right] = \delta_{ik} a_j a^\dagger_l - \delta_{il} a_j a^\dagger_k + \delta_{jk} a^\dagger_l a_i - \delta_{jl} a^\dagger_k a_i.$$

Given an unitary operator $U:\mathcal{H}\to\mathcal{H}$, we obtain an unitary operator (also denoted by U) acting on $\wedge^N\mathcal{H}$ by

$$U\left(\psi_1\wedge\cdots\wedge\psi_N\right) := \left(U\psi_1\right)\wedge\cdots\wedge\left(U\psi_N\right).$$

From

$$\left(U^* a^\dagger_{U\phi} U\right)(\psi_1 \wedge \cdots \wedge \psi_N) = U^*(U\phi \wedge U\psi_1 \wedge \cdots \wedge U\psi_N)$$
$$= \phi \wedge \psi_1 \wedge \cdots \wedge \psi_N$$

we get

$$U^* a^\dagger_{U\phi} U = a^\dagger_\phi$$

for all $\phi \in \mathcal{H}$, and, taking the adjoint,

$$U^* a_{U\phi} U = a_\phi.$$

The canonical generalization to p-body creation and annhihilation operators is as follows:

$$a^\dagger_{i_1\wedge\cdots\wedge i_p + c\cdot j_1\wedge\cdots\wedge j_p} := a^\dagger_{i_1}\cdots a^\dagger_{i_p} + c\cdot a^\dagger_{j_1}\cdots a^\dagger_{j_p},$$
$$a_{i_1\wedge\cdots\wedge i_p + c\cdot j_1\wedge\cdots\wedge j_p} := \left(a^\dagger_{i_1\wedge\cdots\wedge i_p + c\cdot j_1\wedge\cdots\wedge j_p}\right)^*$$
$$= a_{i_p}\cdots a_{i_1} + \bar{c}\cdot a_{j_p}\cdots a_{j_1}.$$

Given $\chi \in \wedge^p\mathcal{H}$, we set

$$\hat{n}_\chi := a^\dagger_\chi a_\chi.$$

This relates to the single-particle occupation numbers as follows:

$$\hat{n}_{i_1\wedge\cdots\wedge i_p} = a^\dagger_{i_1}\cdots a^\dagger_{i_p} a_{i_p}\cdots a_{i_1} = \hat{n}_{i_1}\cdots\hat{n}_{i_p}.$$

For the last expression we have used the anticommutator relations. Let $(\chi_i)_i$ be a complete orthonormal system in $\wedge^p\mathcal{H}$ and fix the particle number $N \geq p$ (that is, we operate on $\wedge^N\mathcal{H}$). Then

$$\sum_i \hat{n}_{\chi_i} = \binom{N}{p}\cdot \mathrm{id}_{\wedge^N\mathcal{H}}.$$

This can be seen by a Slater determinant expansion.

6.3.4 L^2 Wave Functions

In physics, the most widely used Hilbert spaces are L^2 spaces. (And in fact, each finite-dimensional or separable Hilbert space is isomorphic to a L^2 space.) In this chapter we rewrite the creation and annihilation operators in terms of integrals, which are the building blocks of L^2-spaces.

Given a measure space $(\Omega, \mathcal{A}, \mu)$ and $\mathcal{H} = L^2(\Omega, \mathbb{C})$, the wedge product is similar to the antisymmetrized product space, i.e.

$$\begin{aligned} \wedge^N \mathcal{H} \simeq L^2_{\text{anti}}(\Omega^N, \mathbb{C}) :=& \\ \big\{ \Psi \in L^2(\Omega^N, \mathbb{C}) \ | \, \Psi(\dots, x_i, \dots, x_j, \dots) & \\ = \Psi(\dots, x_j, \dots, x_i, \dots) \ \forall i \neq j \ \big\}. \end{aligned}$$

The creation and annihilation operators are given by

$$\begin{aligned} \left(a_\phi^\dagger \Psi\right)(x_1, \dots, x_{N+1}) = \frac{1}{\sqrt{N+1}} \sum_{\alpha=1}^{N+1} (-1)^{\alpha+1} \phi(x_\alpha) \times \\ \Psi(x_1, \dots, x_{\alpha-1}, x_{\alpha+1}, \dots, x_{N+1}) \quad \forall \phi \in \mathcal{H}, \ \Psi \in \wedge^N \mathcal{H} \end{aligned}$$

and

$$\left(a_\phi \Psi\right)(x_1, \dots, x_{N-1}) = \sqrt{N} \int_\Omega \overline{\phi(x)} \Psi(x, x_1, \dots, x_{N-1}) \, \mathrm{d}x.$$

This can be directly derived from the definition. Let $\Psi = \psi_1 \wedge \dots \wedge \psi_N$.

$$\begin{aligned} \left(a_\phi^\dagger \Psi\right) &= \phi \wedge \psi_1 \wedge \dots \wedge \psi_N \\ &= (-1)^N \psi_1 \wedge \dots \wedge \psi_N \wedge \phi \\ &= (-1)^N \frac{1}{\sqrt{N+1}} \sum_{\alpha=1}^{N+1} \phi(x_\alpha) \frac{1}{\sqrt{N!}} \sum_{\substack{\sigma \in S_{N+1} \\ \sigma(\alpha) = N+1}} \operatorname{sgn}(\sigma) \times \\ &\quad \psi_{\sigma(1)}(x_1) \cdots \psi_{\sigma(\alpha-1)}(x_{\alpha-1}) \cdot \psi_{\sigma(\alpha+1)}(x_{\alpha+1}) \cdots \psi_{\sigma(N+1)}(x_{N+1}) \\ &= (-1)^N \frac{1}{\sqrt{N+1}} \sum_{\alpha=1}^{N+1} \phi(x_\alpha) \frac{1}{\sqrt{N!}} (-1)^{N+1-\alpha} \sum_{\tau \in S_N} \operatorname{sgn}(\tau) \times \\ &\quad \psi_{\tau(1)}(x_1) \cdots \psi_{\tau(\alpha-1)}(x_{\alpha-1}) \cdot \psi_{\tau(\alpha)}(x_{\alpha+1}) \cdots \psi_{\tau(N)}(x_{N+1}) \\ &= \frac{1}{\sqrt{N+1}} \sum_{\alpha=1}^{N+1} (-1)^{\alpha+1} \phi(x_\alpha) \Psi(x_1, \dots, x_{\alpha-1}, x_{\alpha+1}, \dots, x_{N+1}). \end{aligned}$$

An explicit calculation based on

$$\left\langle \Psi \,|\, a_\phi^\dagger \Phi \right\rangle = \langle a_\phi \Psi \,|\, \Phi \rangle$$

gives the formula for $a_\phi \Psi$.

Let $\chi = \phi \wedge \psi \in \wedge^2 \mathcal{H}$, then by definition $a_\chi = a_\psi a_\phi$, so

$$\begin{aligned}
(a_\chi \Psi)(x_1, \dots, x_{N-2}) \\
&= \sqrt{N-1} \int_\Omega \overline{\psi(y)} \, (a_\phi \Psi) \, (y, x_1, \dots, x_{N-2}) \, \mathrm{d}y \\
&= \sqrt{N(N-1)} \int_\Omega \int_\Omega \frac{1}{2} \left[\overline{\phi(x)\psi(y) - \phi(y)\psi(x)} \right] \Psi(x, y, x_1, \dots, x_{N-2}) \, \mathrm{d}x \, \mathrm{d}y \\
&= \binom{N}{2}^{\frac{1}{2}} \int_\Omega \int_\Omega \overline{\chi(x,y)} \Psi(x, y, x_1, \dots, x_{N-2}) \, \mathrm{d}x \, \mathrm{d}y.
\end{aligned}$$

A short calculation shows that

$$\begin{aligned}
\left(a_\chi^\dagger \Psi\right)(x_1, \dots, x_{N+2}) = \binom{N+2}{2}^{-\frac{1}{2}} \sum_{\substack{\alpha,\beta=1 \\ \alpha<\beta}}^{N+2} (-1)^{\alpha+\beta+1} \, \chi(x_\alpha, x_\beta) \times \\
\Psi(x_1, \dots, x_{\alpha-1}, x_{\alpha+1}, \dots, x_{\beta-1}, x_{\beta+1}, \dots, x_{N+2}).
\end{aligned}$$

This can easily be generalized to p-body creation and annihilation operators, for example, for $\chi \in \wedge^p \mathcal{H}$ and $\Psi \in \wedge^N \mathcal{H}$,

$$(a_\chi \Psi)(x_1, \dots, x_{N-p}) = \binom{N}{p}^{\frac{1}{2}} \int_{\Omega^p} \overline{\chi(x_1', \dots, x_p')} \Psi(x_1', \dots, x_p', x_1, \dots, x_{N-p}) \, \mathrm{d}x_1' \dots \mathrm{d}x_p'.$$

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