Diagonalization of bosonic quadratic Hamiltonians by Bogoliubov transformations[1]

P. T. Nam[1] **M. Napiórkowski** [1] J. P. Solovej [2]

[1]**Institute of Science and Technology Austria**

[2]Department of Mathematics, University of Copenhagen

GDR Dynqua meeting, Grenoble

[1] *J. Funct. Anal.* (in press)

Bosonic quadratic Hamiltonians on Fock space

General form of quadratic Hamiltonian:

$$\mathbb{H} = \mathrm{d}\Gamma(h) + \frac{1}{2}\sum_{m,n\geq 1}\Big(\langle J^* k f_m, f_n\rangle a(f_m)a(f_n) + \overline{\langle J^* k f_m, f_n\rangle} a^*(f_m)a^*(f_n)\Big)$$

Here:

- a^*/a - **bosonic** creation/annihilation operators (CCR);
- $h > 0$ and $\mathrm{d}\Gamma(h) = \sum_{m,n\geq 1}\langle f_m, h f_n\rangle a^*(f_m)a(f_n)$
- $k : \mathfrak{h} \to \mathfrak{h}^*$ is an (unbounded) linear operator with $D(h) \subset D(k)$ (called *pairing operator*), $k^* = J^* k J^*$;
- $J : \mathfrak{h} \to \mathfrak{h}^*$ is the anti-unitary operator defined by

$$J(f)(g) = \langle f, g\rangle, \quad \forall f, g \in \mathfrak{h}.$$

Bosonic quadratic Hamiltonians on Fock space

General form of quadratic Hamiltonian:

$$\mathbb{H} = \mathrm{d}\Gamma(h) + \frac{1}{2}\sum_{m,n\geq 1}\Big(\langle J^* k f_m, f_n\rangle a(f_m)a(f_n) + \overline{\langle J^* k f_m, f_n\rangle} a^*(f_m)a^*(f_n)\Big)$$

Here:

- a^*/a - **bosonic** creation/annihilation operators (CCR);
- $h > 0$ and $\mathrm{d}\Gamma(h) = \sum_{m,n\geq 1}\langle f_m, h f_n\rangle a^*(f_m)a(f_n)$
- $k : \mathfrak{h} \to \mathfrak{h}^*$ is an (unbounded) linear operator with $D(h) \subset D(k)$ (called *pairing operator*), $k^* = J^* k J^*$;
- $J : \mathfrak{h} \to \mathfrak{h}^*$ is the anti-unitary operator defined by

$$J(f)(g) = \langle f, g\rangle, \quad \forall f, g \in \mathfrak{h}.$$

Operators of that type are important in physics!

- QFT (eg. scalar field with position dependent mass);
- many-body QM (*effective theories* like Bogoliubov or BCS).

The problem

Our goal:
find (prove existence) a unitary transformation $\mathbb{U}$ on the Fock space, such that

$$\mathbb{U}\mathbb{H}\mathbb{U}^* = E + \mathrm{d}\Gamma(\xi).$$

The problem

Our goal:
find (prove existence) a unitary transformation $\mathbb{U}$ on the Fock space, such that

$$\mathbb{U}\mathbb{H}\mathbb{U}^* = E + \mathrm{d}\Gamma(\xi).$$

Why?

- interpretation in terms of a non-interacting theory;
- access to spectral properties of $\mathbb{H}$;
- ...

$$\mathbb{H} = \mathrm{d}\Gamma(h) + \frac{1}{2} \sum_{m,n \geq 1} \Big(\langle J^* k f_m, f_n \rangle a(f_m) a(f_n) + \overline{\langle J^* k f_m, f_n \rangle} a^*(f_m) a^*(f_n) \Big)$$

- **Remark:**
  The above definition is formal! If k is not Hilbert-Schmidt, then it is difficult to show that the domain is dense.

$$\mathbb{H} = \mathrm{d}\Gamma(h) + \frac{1}{2}\sum_{m,n\geq 1}\Big(\langle J^* k f_m, f_n\rangle a(f_m)a(f_n) + \overline{\langle J^* k f_m, f_n\rangle} a^*(f_m)a^*(f_n)\Big)$$

- **Remark:**
  The above definition is formal! If k is not Hilbert-Schmidt, then it is difficult to show that the domain is dense.
- More general approach: **definition through quadratic forms!**
- **One-particle density matrices:** $\gamma_\Psi : \mathfrak{h} \to \mathfrak{h}$ and $\alpha_\Psi : \mathfrak{h} \to \mathfrak{h}^*$

$$\langle f, \gamma_\Psi g\rangle = \langle \Psi, a^*(g)a(f)\Psi\rangle\,, \quad \langle Jf, \alpha_\Psi g\rangle = \langle \Psi, a^*(g)a^*(f)\Psi\rangle\,, \quad \forall f, g \in \mathfrak{h}$$

- A formal calculation leads to the expression

$$\boxed{\langle \Psi, \mathbb{H}\Psi\rangle = \mathrm{Tr}(h^{1/2}\gamma_\Psi h^{1/2}) + \Re\,\mathrm{Tr}(k^*\alpha_\Psi).}$$

Unitary implementability

- Generalized creation and annihilation operators

$$A(f \oplus Jg) = a(f) + a^*(g), \quad A^*(f \oplus Jg) = a^*(f) + a(g), \quad \forall f, g \in \mathfrak{h};$$

- Let $\mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$, bounded;

Definition

A bounded operator $\mathcal{V}$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ is *unitarily implemented* by a unitary operator $\mathbb{U}_{\mathcal{V}}$ on Fock space if

$$\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F), \quad \forall F \in \mathfrak{h} \oplus \mathfrak{h}^*.$$

Unitary implementability

- Generalized creation and annihilation operators

$$A(f \oplus Jg) = a(f) + a^*(g), \quad A^*(f \oplus Jg) = a^*(f) + a(g), \quad \forall f, g \in \mathfrak{h};$$

- Let $\mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \to \mathfrak{h} \oplus \mathfrak{h}^*$, bounded;

Definition

A bounded operator $\mathcal{V}$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ is *unitarily implemented* by a unitary operator $\mathbb{U}_{\mathcal{V}}$ on Fock space if

$$\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F), \quad \forall F \in \mathfrak{h} \oplus \mathfrak{h}^*.$$

- **Our goal:** Find $\mathbb{U}_{\mathcal{V}}$ such that $\mathbb{U}_{\mathcal{V}} \mathbb{H} \mathbb{U}_{\mathcal{V}}^* = E + \mathrm{d}\Gamma(\xi)$.

Quadratic Hamiltonians as quantizations of block operators

Let

$$\mathcal{A} := \begin{pmatrix} h & k^* \\ k & JhJ^* \end{pmatrix}$$

Let

$$\mathcal{A} := \begin{pmatrix} h & k^* \\ k & JhJ^* \end{pmatrix}$$

and

$$\mathbb{H}_{\mathcal{A}} := \frac{1}{2} \sum_{m,n \geq 1} \langle F_m, \mathcal{A} F_n \rangle A^*(F_m) A(F_n).$$

Quadratic Hamiltonians as quantizations of block operators

Let

$$\mathcal{A} := \begin{pmatrix} h & k^* \\ k & JhJ^* \end{pmatrix}$$

and

$$\mathbb{H}_{\mathcal{A}} := \frac{1}{2} \sum_{m,n \geq 1} \langle F_m, \mathcal{A} F_n \rangle A^*(F_m) A(F_n).$$

Then a formal calculation gives

$$\mathbb{H} = \mathbb{H}_{\mathcal{A}} - \frac{1}{2} \operatorname{Tr}(h).$$

Thus, formally, $\mathbb{H}$ can be seen as "quantization" of $\mathcal{A}$.

Diagonalization

If $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$, then

$$\mathbb{U}_{\mathcal{V}} \mathbb{H}_{\mathcal{A}} \mathbb{U}_{\mathcal{V}}^* = \mathbb{H}_{\mathcal{V}\mathcal{A}\mathcal{V}^*}.$$

Diagonalization

If $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$, then

$$\mathbb{U}_{\mathcal{V}} \mathbb{H}_{\mathcal{A}} \mathbb{U}_{\mathcal{V}}^* = \mathbb{H}_{\mathcal{V}\mathcal{A}\mathcal{V}^*}.$$

Thus, if $\mathcal{V}$ diagonalizes $\mathcal{A}$:

$$\mathcal{V}\mathcal{A}\mathcal{V}^* = \begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}$$

for some operator $\xi : \mathfrak{h} \to \mathfrak{h}$, then

$$\mathbb{U}_{\mathcal{V}} \mathbb{H} \mathbb{U}_{\mathcal{V}}^* = \mathbb{U}_{\mathcal{V}} \left(\mathbb{H}_{\mathcal{A}} - \frac{1}{2} \operatorname{Tr}(h) \right) \mathbb{U}_{\mathcal{V}}^* = \mathrm{d}\Gamma(\xi) + \frac{1}{2} \operatorname{Tr}(\xi - h).$$

Diagonalization

If $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$, then

$$\mathbb{U}_{\mathcal{V}} \mathbb{H}_{\mathcal{A}} \mathbb{U}_{\mathcal{V}}^* = \mathbb{H}_{\mathcal{V}\mathcal{A}\mathcal{V}^*}.$$

Thus, if $\mathcal{V}$ diagonalizes $\mathcal{A}$:

$$\mathcal{V}\mathcal{A}\mathcal{V}^* = \begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}$$

for some operator $\xi : \mathfrak{h} \to \mathfrak{h}$, then

$$\mathbb{U}_{\mathcal{V}} \mathbb{H} \mathbb{U}_{\mathcal{V}}^* = \mathbb{U}_{\mathcal{V}} \left(\mathbb{H}_{\mathcal{A}} - \frac{1}{2} \mathrm{Tr}(h) \right) \mathbb{U}_{\mathcal{V}}^* = \mathrm{d}\Gamma(\xi) + \frac{1}{2} \mathrm{Tr}(\xi - h).$$

These formal arguments suggest it is enough to consider the diagonalization of block operators.

Question 1:

Questions

Question 1:

what are the conditions on $\mathcal{V}$ so that $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$?

Questions

Question 1:

what are the conditions on $\mathcal{V}$ so that $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$?

Question 2:

Questions

Question 1:

what are the conditions on $\mathcal{V}$ so that $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^{*} = A(\mathcal{V}F)$?

Question 2:

what are the conditions on $\mathcal{A}$ so that there exists a $\mathcal{V}$ that diagonalizes $\mathcal{A}$?

Question 1 - symplectic transformations

Recall $A(f \oplus Jg) = a(f) + a^*(g)$ and $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$.

- Conjugate and canonical commutation relations:

$$A^*(F_1) = A(\mathcal{J}F_1), \quad [A(F_1), A^*(F_2)] = (F_1, \mathcal{S}F_2), \quad \forall F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*$$

where

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathcal{J} = \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix}.$$

Question 1 - symplectic transformations

Recall $A(f \oplus Jg) = a(f) + a^*(g)$ and $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$.

- Conjugate and canonical commutation relations:

$$A^*(F_1) = A(\mathcal{J}F_1), \quad [A(F_1), A^*(F_2)] = (F_1, \mathcal{S}F_2), \quad \forall F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*$$

  where

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathcal{J} = \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix}.$$

- $S = S^{-1} = S^*$ is unitary, $\mathcal{J} = \mathcal{J}^{-1} = \mathcal{J}^*$ is anti-unitary.
- Compatibility (wrt implementability) conditions

$$\mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V}, \quad \mathcal{V}^* S \mathcal{V} = S = \mathcal{V} S \mathcal{V}^*. \tag{1}$$

- Any bounded operator $\mathcal{V}$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ satisfying (1) is called a *symplectic transformation*.

Question 1 - implementability

- Symplecticity of $\mathcal{V}$ implies

$$\mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V} \qquad \Rightarrow \qquad \mathcal{V} = \begin{pmatrix} U & J^* V J^* \\ V & J U J^* \end{pmatrix}$$

Question 1 - implementability

- Symplecticity of $\mathcal{V}$ implies

$$\mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V} \qquad \Rightarrow \qquad \mathcal{V} = \begin{pmatrix} U & J^* V J^* \\ V & J U J^* \end{pmatrix}$$

Fundamental result:

Shale's theorem ('62)

A symplectic transformation $\mathcal{V}$ is unitarily implementable (i.e. $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$), if and only if

$$\|V\|_{\mathrm{HS}}^2 = \mathrm{Tr}(V^* V) < \infty.$$

Question 1 - implementability

- Symplecticity of $\mathcal{V}$ implies

$$\mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V} \qquad \Rightarrow \qquad \mathcal{V} = \begin{pmatrix} U & J^* V J^* \\ V & J U J^* \end{pmatrix}$$

Fundamental result:

Shale's theorem ('62)

A symplectic transformation $\mathcal{V}$ is unitarily implementable (i.e. $\mathbb{U}_\mathcal{V} A(F) \mathbb{U}_\mathcal{V}^* = A(\mathcal{V}F)$), if and only if

$$\|V\|_{\mathrm{HS}}^2 = \mathrm{Tr}(V^* V) < \infty.$$

$\mathbb{U}_\mathcal{V}$, a unitary implementer on the Fock space of a symplectic transformation $\mathcal{V}$, is called a *Bogoliubov transformation*.

Question 2 - example: commuting operators in ∞ dim

- $h > 0$ and $k = k^*$ be commuting operators on $\mathfrak{h} = L^2(\Omega, \mathbb{C})$
- $$\mathcal{A} := \begin{pmatrix} h & k \\ k & h \end{pmatrix} > 0 \quad \text{on } \mathfrak{h} \oplus \mathfrak{h}^*.$$
  if and only if $G < 1$ with $G := |k| h^{-1}$.
- $\mathcal{A}$ is diagonalized by the linear operator
  $$\mathcal{V} := \sqrt{\frac{1}{2} + \frac{1}{2\sqrt{1-G^2}}} \begin{pmatrix} 1 & \frac{-G}{1+\sqrt{1-G^2}} \\ \frac{-G}{1+\sqrt{1-G^2}} & 1 \end{pmatrix}$$
  in the sense that
  $$\mathcal{V}\mathcal{A}\mathcal{V}^* = \begin{pmatrix} \xi & 0 \\ 0 & \xi \end{pmatrix} \quad \text{with} \quad \xi := h\sqrt{1-G^2} = \sqrt{h^2 - k^2} > 0.$$
- $\mathcal{V}$ satisfies the compatibility conditions and is bounded (and hence a symplectic transformation) iff $\|G\| = \|kh^{-1}\| < 1$
- $\mathcal{V}$ is unitarily implementable iff kh^{-1} is Hilbert-Schmidt.

Historical remarks

- For $\dim \mathfrak{h} < \infty$ this follows from Williamson's Theorem ('36);
- Friedrichs ('50s) and Berezin ('60s): $h \geq \mu > 0$ bounded with gap and k Hilbert-Schmidt;
- Grech-Seiringer ('13): $h > 0$ with compact resolvent, k Hilbert-Schmidt;
- Lewin-Nam-Serfaty-Solovej ('15): $h \geq \mu > 0$ unbounded, k Hilbert-Schmidt;
- Bach-Bru ('16): $h > 0$, $\|kh^{-1}\| < 1$ and kh^{-s} is Hilbert-Schmidt for all $s \in [0, 1+\epsilon]$ for some $\epsilon > 0$.
- **Our result:** essentially optimal conditions

Theorem [Diagonalization of block operators]

(i) (Existence). Let $h : \mathfrak{h} \to \mathfrak{h}$ and $k : \mathfrak{h} \to \mathfrak{h}^*$ be (unbounded) linear operators satisfying $h = h^* > 0$, $k^* = J^* k J^*$ and $D(h) \subset D(k)$. Assume that the operator $G := h^{-1/2} J^* k h^{-1/2}$ is densely defined and extends to a bounded operator satisfying $\|G\| < 1$. Then we can define the self-adjoint operator

$$\mathcal{A} := \begin{pmatrix} h & k^* \\ k & JhJ^* \end{pmatrix} > 0 \quad \text{on } \mathfrak{h} \oplus \mathfrak{h}^*$$

by Friedrichs' extension. This operator can be diagonalized by a symplectic transformation $\mathcal{V}$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ in the sense that

$$\mathcal{V}\mathcal{A}\mathcal{V}^* = \begin{pmatrix} \xi & 0 \\ 0 & J\xi J^* \end{pmatrix}$$

for a self-adjoint operator $\xi > 0$ on $\mathfrak{h}$. Moreover, we have

$$\|\mathcal{V}\| \le \left(\frac{1 + \|G\|}{1 - \|G\|} \right)^{1/4}.$$

Theorem [Diagonalization of block operators]

(ii) (Implementability). Assume further that G is Hilbert-Schmidt. Then $\mathcal{V}$ is unitarily implementable and

$$\|V\|_{\mathrm{HS}} \leq \frac{2}{1-\|G\|}\|G\|_{\mathrm{HS}}.$$

Theorem [Diagonalization of quadratic Hamiltonians]

Recall $G := h^{-1/2} J^* k h^{-1/2}$. Assume, as before, that $\|G\| < 1$ and G is Hilbert-Schmidt. Assume further that $kh^{-1/2}$ is Hilbert-Schmidt. Then the quadratic Hamiltonian $\mathbb{H}$, defined before as a quadratic form, is bounded from below and closable, and hence its closure defines a self-adjoint operator which we still denote by $\mathbb{H}$. Moreover, if $\mathbb{U}_{\mathcal{V}}$ is the unitary operator on Fock space implementing the symplectic transformation $\mathcal{V}$, then

$$\mathbb{U}_{\mathcal{V}} \mathbb{H} \mathbb{U}_{\mathcal{V}}^* = \mathrm{d}\Gamma(\xi) + \inf \sigma(\mathbb{H})$$

and

$$\inf \sigma(\mathbb{H}) \geq -\frac{1}{2} \|kh^{-1/2}\|_{\mathrm{HS}}^2.$$

Sketch of proof

Step 1. - fermionic case. If B is a self-adjoint and such that $\mathcal{J}B\mathcal{J} = -B$, then there exists a unitary operator $\mathcal{U}$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ such that $\mathcal{J}\mathcal{U}\mathcal{J} = \mathcal{U}$ and

$$\mathcal{U}B\mathcal{U}^* = \begin{pmatrix} \xi & 0 \\ 0 & -J\xi J^* \end{pmatrix}.$$

Sketch of proof

Step 1. - fermionic case. If B is a self-adjoint and such that $\mathcal{J}B\mathcal{J} = -B$, then there exists a unitary operator $\mathcal{U}$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ such that $\mathcal{J}\mathcal{U}\mathcal{J} = \mathcal{U}$ and

$$\mathcal{U}B\mathcal{U}^* = \begin{pmatrix} \xi & 0 \\ 0 & -J\xi J^* \end{pmatrix}.$$

Step 2. Apply Step 1 to $B = \mathcal{A}^{1/2} S \mathcal{A}^{1/2}$.

Sketch of proof

Step 1. - fermionic case. If B is a self-adjoint and such that $\mathcal{J} B \mathcal{J} = -B$, then there exists a unitary operator $\mathcal{U}$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ such that $\mathcal{J} \mathcal{U} \mathcal{J} = \mathcal{U}$ and

$$\mathcal{U} B \mathcal{U}^* = \begin{pmatrix} \xi & 0 \\ 0 & -J \xi J^* \end{pmatrix}.$$

Step 2. Apply Step 1 to $B = \mathcal{A}^{1/2} S \mathcal{A}^{1/2}$.

Step 3. Explicit construction of the symplectic transformation $\mathcal{V}$:

$$\mathcal{V} := \mathcal{U} |B|^{1/2} \mathcal{A}^{-1/2}.$$

Sketch of proof

Step 1. - fermionic case. If B is a self-adjoint and such that $\mathcal{J}B\mathcal{J} = -B$, then there exists a unitary operator $\mathcal{U}$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ such that $\mathcal{J}\mathcal{U}\mathcal{J} = \mathcal{U}$ and

$$\mathcal{U}B\mathcal{U}^* = \begin{pmatrix} \xi & 0 \\ 0 & -J\xi J^* \end{pmatrix}.$$

Step 2. Apply Step 1 to $B = \mathcal{A}^{1/2}S\mathcal{A}^{1/2}$.

Step 3. Explicit construction of the symplectic transformation $\mathcal{V}$:

$$\mathcal{V} := \mathcal{U}|B|^{1/2}\mathcal{A}^{-1/2}.$$

Step 4. A detailed study of $\mathcal{V}^*\mathcal{V} = \mathcal{A}^{-1/2}|B|\mathcal{A}^{-1/2}$.

Thank you for your attention!