Diagonalization of bosonic quadratic Hamiltonians by Bogoliubov transformations

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Bosonic quadratic Hamiltonians on Fock space

General form of quadratic Hamiltonian:

\[ \mathcal{H} = d\Gamma(h) + \frac{1}{2} \sum_{m,n \geq 1} \left( \langle J^* k f_m, f_n \rangle a(f_m) a(f_n) + \langle J^* k f_m, f_n \rangle a^*(f_m) a^*(f_n) \right) \]

Here:

- \( a^*/a \) - bosonic creation/annihilation operators (CCR);
- \( h > 0 \) and \( d\Gamma(h) = \sum_{m,n \geq 1} \langle f_m, hf_n \rangle a^*(f_m) a(f_n) \);
- \( k : \mathfrak{h} \to \mathfrak{h}^* \) 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
  \[ J(f)(g) = \langle f, g \rangle, \quad \forall f, g \in \mathfrak{h}. \]
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▶ \(k : \mathfrak{h} \to \mathfrak{h}^*\) is an (unbounded) linear operator with \(D(h) \subset D(k)\) (called **pairing operator**), \(k^* = J^* k J^*\);
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\[ J(f)(g) = \langle f, g \rangle, \quad \forall f, g \in \mathfrak{h}. \]

**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).
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Why?

- interpretation in terms of a non-interacting theory;
- access to spectral properties of $\mathcal{H}$;
- ...
\[ \mathcal{H} = d\Gamma(h) + \frac{1}{2} \sum_{m,n \geq 1} \left( \langle J^* k f_m, f_n \rangle a(f_m) a(f_n) + \langle J^* k f_m, f_n \rangle a^*(f_m) a^*(f_n) \right) \]

**Remark:**

The above definition is **formal**! If \( k \) is not Hilbert-Schmidt, then it is difficult to show that the domain is dense.
\[ \mathcal{H} = d\Gamma(h) + \frac{1}{2} \sum_{m,n \geq 1} \left( \langle J^* k f_m, f_n \rangle a(f_m)a(f_n) + \langle J^* k f_m, f_n \rangle a^*(f_m)a^*(f_n) \right) \]

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**More general approach:** definition through quadratic forms!

**One-particle density matrices:** \( \gamma_\Psi : \mathfrak{h} \rightarrow \mathfrak{h} \) and \( \alpha_\Psi : \mathfrak{h} \rightarrow \mathfrak{h}^* \)

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

**A formal calculation leads to the expression**

\[ \langle \Psi, \mathcal{H}\Psi \rangle = \text{Tr}(h^{1/2}\gamma_\Psi h^{1/2}) + \Re \text{Tr}(k^* \alpha_\Psi). \]
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 \( \mathcal{V} : \mathfrak{h} \oplus \mathfrak{h}^* \rightarrow \mathfrak{h} \oplus \mathfrak{h}^* \), bounded;

**Definition**

A bounded operator \( \mathcal{V} \) on \( \mathfrak{h} \oplus \mathfrak{h}^* \) is *unitarily implemented* by a unitary operator \( U_{\mathcal{V}} \) on Fock space if

\[ U_{\mathcal{V}} A(F) U_{\mathcal{V}}^* = A(\mathcal{V} F), \quad \forall F \in \mathfrak{h} \oplus \mathfrak{h}^*. \]
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**Our goal:** Find \( U_{\mathcal{V}} \) such that \( U_{\mathcal{V}} H U_{\mathcal{V}}^* = E + d\Gamma(\xi) \).
Let

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Then a formal calculation gives

\[ \mathbb{H} = \mathbb{H}_A - \frac{1}{2} \text{Tr}(h). \]

Thus, formally, \( \mathbb{H} \) can be seen as "quantization" of \( A \).
If $U_{\mathcal{V}} A(F) U_{\mathcal{V}}^* = A(\mathcal{V} F)$, then

$$U_{\mathcal{V}} H A U_{\mathcal{V}}^* = H_{\mathcal{V}} A_{\mathcal{V}}^*.$$
Diagonalization

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

\[
U \mathcal{V} \mathcal{H} \mathcal{A} U^* = \mathcal{H} \mathcal{V} A \mathcal{V}^*.
\]

Thus, if \( \mathcal{V} \) diagonalizes \( \mathcal{A} \):

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

for some operator \( \xi : \mathfrak{h} \rightarrow \mathfrak{h} \), then

\[
U \mathcal{V} \mathcal{H} U^* = U \mathcal{V} \left( \mathcal{H} \mathcal{A} - \frac{1}{2} \text{Tr}(h) \right) U^* = d \Gamma(\xi) + \frac{1}{2} \text{Tr}(\xi - h).
\]
If $U_{\mathcal{V}} A(F) U_{\mathcal{V}}^* = A(V F)$, then

$$U_{\mathcal{V}} H_{\mathcal{A}} U_{\mathcal{V}}^* = H_{\mathcal{V}} A_{\mathcal{V}}^*.$$ 

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

$$\mathcal{V} A_{\mathcal{V}}^* = \left( \begin{array}{cc} \xi & 0 \\ 0 & J \xi J^* \end{array} \right)$$

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

$$U_{\mathcal{V}} H U_{\mathcal{V}}^* = U_{\mathcal{V}} \left( H_{\mathcal{A}} - \frac{1}{2} \text{Tr}(h) \right) U_{\mathcal{V}}^* = d\Gamma(\xi) + \frac{1}{2} \text{Tr}(\xi - h).$$

These formal arguments suggest it is enough to consider the diagonalization of block operators.
Question 1:

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

Question 2:

what are the conditions on $A$ so that there exists a $V$ that diagonalizes $A$?
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what are the conditions on $A$ so that there exists a $\mathcal{V}$ that diagonalizes $A$?
Recall \( A(f \oplus Jg) = a(f) + a^*(g) \) and \( U_V A(F) U^*_V = A(VF) \).

- Conjugate and canonical commutation relations:

\[
A^*(F_1) = A(JF_1), \quad \left[ A(F_1), A^*(F_2) \right] = (F_1, SF_2), \quad \forall F_1, F_2 \in \mathfrak{h} \oplus \mathfrak{h}^*
\]

where

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

- $S = S^{-1} = S^*$ is unitary, $J = J^{-1} = J^*$ is anti-unitary.

- Compatibility (wrt implementability) conditions

$$J\mathcal{V}J = \mathcal{V}, \quad \mathcal{V}^*SV = S = \mathcal{V}SV^*. \quad \text{(1)}$$

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

$$\mathcal{J}\mathcal{V}\mathcal{J} = \mathcal{V} \quad \Rightarrow \quad \mathcal{V} = \begin{pmatrix} U & J^* V J^* \\ V & J U J^* \end{pmatrix}$$
Question 1 - implementability

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**Fundamental result:**

**Shale’s theorem (’62)**

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

\[ \|V\|_{\text{HS}}^2 = \text{Tr}(V^*V) < \infty. \]
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\]

$U_{\mathcal{V}}$, a unitary implementer on the Fock space of a symplectic transformation $\mathcal{V}$, is called a **Bogoliubov transformation**.
Question 2 - example: commuting operators in $\infty$ dim

$\mathbf{h} > 0$ and $k = k^*$ be commuting operators on $\mathfrak{h} = L^2(\Omega, \mathbb{C})$

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

if and only if $G < 1$ with $G := |k| h^{-1}$.

$A$ is diagonalized by the linear operator

$V := \sqrt{\frac{1}{2} + \frac{1}{2\sqrt{1-G^2}}} \begin{pmatrix} 1 & -G \\ -G & \sqrt{1-G^2} \end{pmatrix}$

in the sense that

$VAV^* = \begin{pmatrix} \xi & 0 \\ 0 & \xi \end{pmatrix}$ with $\xi := h \sqrt{1-G^2} = \sqrt{h^2 - k^2} > 0$.

$V$ satisfies the compatibility conditions and is bounded (and hence a symplectic transformation) iff $\|G\| = \|kh^{-1}\| < 1$.

$V$ 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-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
(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

$$\|\mathcal{V}\| \leq \left( \frac{1 + \|G\|}{1 - \|G\|} \right)^{1/4}.$$
(ii) (Implementability). Assume further that $G$ is Hilbert-Schmidt. Then $\mathcal{V}$ is unitarily implementable and

$$\|V\|_{\text{HS}} \leq \frac{2}{1 - \|G\|_{\text{HS}}} \|G\|_{\text{HS}}.$$
Theorem [Diagonalization of quadratic Hamiltonians]

Recall $G := h^{-1/2}J^*kh^{-1/2}$. 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 $U_\mathcal{V}$ is the unitary operator on Fock space implementing the symplectic transformation $\mathcal{V}$, then

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

and

$$\inf \sigma(\mathbb{H}) \geq -\frac{1}{2}\|kh^{-1/2}\|_{\text{HS}}^2.$$
Step 1. - fermionic case. If $B$ is a self-adjoint and such that $JBJ = -B$, then there exists a unitary operator $U$ on $\mathfrak{h} \oplus \mathfrak{h}^*$ such that $JUJ = U$ and

$$UBU^* = \begin{pmatrix} \xi & 0 \\ 0 & -J\xi J^* \end{pmatrix}.$$
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Quadratic Hamiltonians and Bogoliubov transformations
Sketch of proof

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

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

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

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Thank you for your attention!