Bosonic quadratic Hamiltonians and their diagonalization

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"Macroscopic Limits of Quantum Systems"
70th Birthday of Herbert Spohn

Main object of interest:

$$\mathbb{H} = \sum_{ij} h_{ij} a_i^* a_j + \frac{1}{2} \sum_{ij} k_{ij} a_i^* a_j^* + \frac{1}{2} \sum_{ij} \overline{k}_{ij} a_i a_j$$

Here:

- h_{ij} is a self-adjoint matrix ($h_{ij} = h_{ij}^* = \overline{h}_{ij}^{\#}$);
- $\overline{k}_{ij}$ is the complex conjugate of the matrix k_{ij};
- a_i^*/a_i are the bosonic creation/annihilation operators on the Fock space:

$$[a_i^*, a_j^*] = [a_i, a_j] = 0, \qquad [a_i, a_j^*] = \delta_{ij};$$

- the sum might be over an infinite set of indices.

Operators of that type are important in physics!

1. they appear as **effective theories** for quantum many-body systems. Examples:
   - Bogoliubov theory for bosonic systems
   - BCS theory (and BCS-like theories) for fermionic systems
2. quantum field theory (eg. scalar field with position dependent mass).

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Bogoliubov theory: (describes low-energy behaviour of bosonic systems)

$$\mathbb{H}_{\text{Bog}} = \sum_{p\neq 0} p^2 a_p^* a_p + \frac{\rho}{2} \sum_{p\neq 0} \underbrace{\widehat{w}(p)}_{>0} (2a_p^* a_p + a_p^* a_{-p}^* + a_p a_{-p})$$

Question: what are the spectral properties of this operator?

$\Rightarrow$ DIAGONALIZATION:

$$\boxed{\mathbb{U}\mathbb{H}_{\text{Bog}}\mathbb{U} = \tilde{\mathbb{H}}_{\text{Bog}} = E + \sum e(p) b_p^* b_p}$$

Diagonalization of Bogoliubov Hamiltonian

Introduce

$$a_p^* = u_p b_p^* + v_{-p} b_{-p}, \qquad [b_p, b_{p'}^*] = \delta_{pp'} \quad \text{(CCR)}.$$

In particular:

$$\text{(CCR)} \;\Rightarrow\; u_p^2 - v_{-p}^2 = 1 \;\Rightarrow\; u_p = \cosh(\alpha_p), v_{-p} = \sinh(\alpha_p)$$

Diagonalization condition:

$b_p^* b_{-p}^*$ and $b_p b_{-p}$ terms vanish if $\frac{\rho \hat{w}(p)}{2} \underbrace{(u_p^2 + v_{-p}^2)}_{\cosh(2\alpha_p)} + (p^2 + \rho \hat{w}(p)) \underbrace{u_p v_{-p}}_{\frac{1}{2}\sinh 2\alpha_p} = 0$

which yields $\coth(2\alpha_p) = -\frac{p^2 + \rho \hat{w}(p)}{\rho \hat{w}(p)}$ and

$$\Rightarrow \qquad \boxed{\tilde{\mathbb{H}}_{\text{Bog}} = E + \sum_{p \neq 0} e(p) b_p^* b_p}$$

with $e(p) = \sqrt{p^4 + 2\rho \widehat{w}(p) p^2}$.

Question:

When, in general, can $\mathbb{H}$ be diagonalized?

We saw a 2-dimensional example. Finite dimensional case solved (essentially due to Williamson's Theorem on symplectic transformations '36). **What about infinite dimension?**

Fock space formalism

- Fock space:

$$\mathcal{F}(\mathfrak{h}) := \bigoplus_{N=0}^{\infty} \bigotimes_{\text{sym}}^{N} \mathfrak{h} = \mathbb{C} \oplus \mathfrak{h} \oplus (\mathfrak{h} \otimes_s \mathfrak{h}) \oplus \cdots$$

- Creation and anihilation operators:

$$a^*(f_{N+1}) \left(\sum_{\sigma \in S_N} f_{\sigma(1)} \otimes \ldots \otimes f_{\sigma(N)} \right) = \frac{1}{\sqrt{N+1}} \sum_{\sigma \in S_{N+1}} f_{\sigma(1)} \otimes \ldots \otimes f_{\sigma(N+1)},$$

$$a(f_{N+1}) \left(\sum_{\sigma \in S_N} f_{\sigma(1)} \otimes \ldots \otimes f_{\sigma(N)} \right) = N^{\frac{1}{2}} \sum_{\sigma \in S_N} \langle f_{N+1}, f_{\sigma(1)} \rangle f_{\sigma(2)} \otimes \ldots \otimes f_{\sigma(N
$$

for all $f_1, \ldots, f_{N+1}$ in $\mathfrak{h}$, and all $N = 0, 1, 2, \ldots$

- Canonical commutation relations:

$$[a(f), a(g)] = 0, \quad [a^*(f), a^*(g)] = 0, \quad [a(f), a^*(g)] = \langle f, g \rangle, \quad \forall f, g \in \mathfrak{h}.$$

Fock space formalism

Assume $h > 0$. Recall:

$$\mathrm{d}\Gamma(h) = \sum_{m,n\geq 1} \langle f_m, h f_n\rangle a^*(f_m) a(f_n)$$

where $\{f_n\}_{n\geq 1} \subset D(h)$ is an arbitrary orthonormal basis for $\mathfrak{h}$.

General form of quadratic operator:

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

Here:

- $k : \mathfrak{h} \to \mathfrak{h}^*$ 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

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

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

- **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

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

- <u>**Definition:**</u> 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

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

- General form of the transformation we have seen:
  Pick $F = f \oplus 0$. Then $A(F) = a(f)$.

  But $\mathcal{V}F = f_1 \oplus Jf_2$ and thus $A(\mathcal{V}F) = a(f_1) + a^*(f_2)$.

  We get:

$$\mathbb{U}_\mathcal{V} A(F) \mathbb{U}_\mathcal{V}^* = \underbrace{\mathbb{U}_\mathcal{V} a(f) \mathbb{U}_\mathcal{V}^*}_{=:\, b(f)} = A(\mathcal{V}F) = a(f_1) + a^*(f_2).$$

Quadratic Hamiltonians as quantizations of block operators

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

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

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

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

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

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

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

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

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

- 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

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

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 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 bounded and $\|G\| < 1$. 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

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

Theorem [Diagonalization of block operators]

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

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

(ii) (Boundedness from below). 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

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

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

Step 4a. If $\mathcal{V}^*\mathcal{V} - 1$ is Hilbert-Schmidt, then $\mathcal{V}$ is implementable.

Step 4b. Using functional calculus

$$\mathcal{V}^*\mathcal{V} - 1 = \frac{1}{\pi}\int_0^\infty \frac{1}{t+\mathcal{A}^2}\underbrace{(S\mathcal{A}S - \mathcal{A})}_{=:\,E}\mathcal{A}^{1/2}\frac{1}{t+B^2}\mathcal{A}^{-1/2}\sqrt{t}dt.$$

Then use Cauchy-Schwarz with

$$X := \frac{1}{t+\mathcal{A}^2}E\mathcal{A}^{1/2}|B|^{-1}, \quad Y := |B|\frac{1}{t+B^2}\mathcal{A}^{-1/2}.$$

This gives

$$\pm 2(\mathcal{V}^*\mathcal{V} - 1) \le \epsilon^{-1}K + \epsilon\mathcal{A}^{-1/2}|B|\mathcal{A}^{-1/2} = \epsilon^{-1}K + \epsilon\mathcal{V}^*\mathcal{V}$$

where

$$K := \frac{2}{\pi}\int_0^\infty \frac{1}{t+\mathcal{A}^2}ES\mathcal{A}^{-1}SE\frac{1}{t+\mathcal{A}^2}\sqrt{t}dt.$$

Step 4c. We rewrite

$$\pm 2(\mathcal{V}^*\mathcal{V} - 1) \leq \epsilon^{-1} K + \epsilon \mathcal{V}^*\mathcal{V} \leq \epsilon^{-1} K + C\epsilon.$$

Step 4d. $\operatorname{Tr} K < \infty$.

Step 4e. Lemma: If $L = L^*$ boundedand there exists a trace class operator $K \geq 0$ such that

$$\pm 2L \leq \epsilon^{-1} K + \epsilon, \quad \forall \epsilon > 0,$$

then L is Hilbert-Schmidt and $\|L\|_{\mathrm{HS}}^2 \leq \operatorname{Tr}(K)$.

Thank you for your attention
and, last but not least,

HAPPY BIRTHDAY HERBERT!