Density Operators and the Uncertainty Principle

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Maurice de Gosson

University of Vienna-NuHAG

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The Density Operator

Let $\mathcal{H}$ be a Hilbert space. A density operator on $\mathcal{H}$ is a bounded operator $\widehat{\rho} : \mathcal{H} \longrightarrow \mathcal{H}$ having the three following properties:

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- *It is the last property which causes problems, because the condition $\widehat{\rho} \geq 0$ usually holds for some values of $\hbar$ and is violated for others...*

The Density Operator

It follows from the spectral theorem for compact operators that there exist normalized functions $\psi_1, \psi_2, \ldots$ in $\mathcal{H}$ such that

$$\widehat{\rho} = \sum_j \alpha_j P_j \quad \text{with } \alpha_j \geq 0 \text{ and } \sum_j \alpha_j = 1$$

where P_j is the orthogonal projection of the ray generated by ψ_j, that is $P_j \phi = \left\langle \psi_j | \phi \right\rangle \psi_j$.
The operator $\widehat{\rho}$ is the density operator of the mixed state $\psi = \sum_j \alpha_j \psi_j$.
The average (mean value) of an operator $\widehat{A}$ (or "observable") is given by the formula

$$\left\langle \widehat{A} \right\rangle_{\widehat{\rho}} = \mathrm{Tr}(\widehat{A}\widehat{\rho}).$$

Density Operator and Wigner Distribution

We now assume $\mathcal{H} = L^2(\mathbb{R}^n)$.

- The operator kernel of the density operator $\widehat{\rho} = \sum_j \alpha_j P_j$ is $K_{\widehat{\rho}} = \sum_j \alpha_j \psi_j \otimes \psi_j^*$ hence we can write $\widehat{\rho}$ as a Weyl pseudodifferential operator

$$\widehat{\rho}\psi(x) = \iint_{\mathbb{R}^n \times \mathbb{R}^n} e^{\frac{i}{\hbar} p\cdot(x-y)} \rho(\tfrac{1}{2}(x+y), p)\psi(y)dydp.$$

where ρ is the *Wigner distribution* of $\widehat{\rho}$:

$$\rho(x,p) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar} p\cdot y} K_{\widehat{\rho}}(x + \tfrac{1}{2}y, x - \tfrac{1}{2}y)dy \ .$$

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- Equivalently: $\rho(x,p) = \sum_j \alpha_j W\psi_j(x,p)$ where

$$W\psi_j(x,p) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar} p\cdot y} \psi_j(x + \tfrac{1}{2}y)\psi_j^*(x - \tfrac{1}{2}y)dy$$

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- The condition $\operatorname{Tr}\widehat{\rho} = 1$ is equivalent to $\int_{\mathbb{R}^n \times \mathbb{R}^n} \rho(x,p)dpdx = 1$.

Density operator and Wigner Distribution for Physicists!

If you *really* insist on preferring bra-ket notation:
The density operator can be written as

$$\widehat{\rho} = \sum_j \alpha_j \left|\psi_j\right\rangle \left\langle\psi_j\right|.$$

and

$$\rho(x,p) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^n} \left\langle x + \tfrac{1}{2}y\right| \widehat{\rho} \left|x - \tfrac{1}{2}y\right\rangle dy.$$

Also: the kernel can be rewritten:

$$\langle y| \widehat{\rho} |x\rangle = \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}(y-x)\cdot p} \rho\left(\tfrac{1}{2}(x+y), p\right) dp.$$

Density operator and Weyl–Heisenberg Operators

- Let $z = (x, p)$ and $z' = (x', p')$. The symplectic Fourier $\rho_\sigma^\hbar = \mathcal{F}_\sigma \rho$ transform of the Wigner distribution ρ of $\widehat{\rho}$ is defined by

$$\rho_\sigma^\hbar(z) = \left(\tfrac{1}{2\pi\hbar}\right)^n \int_{\mathbb{R}^{2n}} e^{-\frac{i}{\hbar}\sigma(z,z')}\rho(z')dz'$$

where $\sigma(z; z') = p \cdot x' - p' \cdot x$ is the standard symplectic form. Notice that the condition $\mathrm{Tr}\,\widehat{\rho} = 1$ is equivalent to $\rho_\sigma^\hbar(0) = \left(\tfrac{1}{2\pi\hbar}\right)^n$.

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- We then have the beautiful formula

$$\widehat{\rho} = \int_{\mathbb{R}^{2n}} \rho_\sigma^\hbar(z_0)\widehat{T}^\hbar(z_0)dz_0$$

  where $\widehat{T}^\hbar(z_0)$ is the Heisenberg–Weyl operator:

$$\widehat{T}^\hbar(z_0)\psi(x) = e^{\frac{i}{\hbar}(p_0 \cdot x - \frac{1}{2}p_0 \cdot x_0)}\psi(x - x_0).$$

Positivity and Uncertainty Principle

- The positivity of a density operator is related to the *uncertainty principle* of quantum mechanics in its strong (Robertson–Schrödinger) form. This principle can be stated as follows: let $\widehat{\rho}$ be a putative density operator. Then

$$(\Delta X_j)^2_{\widehat{\rho}}(\Delta P_j)^2_{\widehat{\rho}} \geq [\mathrm{Cov}(X_j, P_j)_{\widehat{\rho}}]^2 + \tfrac{1}{4}\hbar^2$$

where, by definition,

$$(\Delta X_j)^2_{\widehat{\rho}} = \left\langle X_j^2 \right\rangle_{\widehat{\rho}} - \langle X_j \rangle^2_{\widehat{\rho}} \quad , \quad (\Delta P_j)^2_{\widehat{\rho}} = \left\langle P_j^2 \right\rangle_{\widehat{\rho}} - \langle P_j \rangle^2_{\widehat{\rho}}$$

and

$$\mathrm{Cov}(X_j, P_j)_{\widehat{\rho}} = \int_{\mathbb{R}^{2n}} (x_j - \langle x_j \rangle_\rho)(x_k - \langle x_k \rangle_\rho)\rho(z)dz.$$

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- The condition $\widehat{\rho} \geq 0$ implies the UP.
- However: *the UP is not sufficient to ensure that* $\widehat{\rho} \geq 0$!

Positivity and UP

...here is a counterexample due to Narcowich: take for simplicity $\hbar = 1$ and choose

$$\rho_\sigma(x, p) = (1 - \tfrac{1}{2}\alpha x^2 - \tfrac{1}{2}\beta p^2) e^{-(\alpha^2 x^4 + \beta^2 p^4)} \quad , \quad \alpha, \beta > 0.$$

One verifies that although the uncertainty relations are satisfied we have

$$\langle P^4 \rangle_{\widehat{\rho}} = \int_{\mathbb{R}^2} p^4 \rho(x, p) dxdp = -24\alpha^2 < 0$$

so that $\widehat{\rho}$ is not positive semi-definite! So the UP is not a sufficient condition for a self-adjoint operator with trace one to be a density operator.

Positivity and the KLM conditions

- It turns out that the "true" conditions ensuring positive semi-definiteness are known in mathematics; they are the KLM (Kastler, Loupias, Miracle-Sole) conditions. Defining the $\hbar = 1$ symplectic Fourier transform $\rho_\sigma(z) = \rho_\sigma^{\hbar=1}(z)$the KLM conditions can be stated in the following way:

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- For *any* sequence $z_1, ..., z_N$ of phase space points $z_j = (x_j, p_j)$ the Hermitian $N \times N$ operator $M^\hbar = (M_{jk}^\hbar)_{1 \leq j,k \leq N}$ with (j, k) entry

$$M_{jk}^\hbar = \rho_\sigma(z_j - z_k) e^{-i\hbar\sigma(z_j, z_k)}$$

is *positive-definite*, that is

$$\sum_{1 \leq j,k \leq N} \rho_\sigma(z_j - z_k) e^{-\frac{i}{2}\hbar\sigma(z_j, z_k)} \lambda_j \lambda_k^* \geq 0$$

for all complex numbers $\lambda_1, ..., \lambda_N$. (We assume from now on that ρ_σ is continuous).

Positivity and the KLM conditions

The KLM conditions serve to clarify the connection between classical and quantum states. When $\hbar = 0$ the KLM conditions reduce to the condition for ρ_σ to be a function of positive type:

$$\sum_{1 \leq j,k \leq N} \rho_\sigma(z_j - z_k)\lambda_j \lambda_k^* \geq 0.$$

By Bochner's theorem ρ_σ is then the (symplectic) Fourier transform of a non-negative finite measure on phase space, that is, of a *classical state*.

Example

Suppose that $\widehat{\rho}$ is the density operator of a pure state: $\rho = W\psi$. Then $\widehat{\rho} > 0$ (strict inequality!) if and only if ψ is a Gaussian: this is the famous "Hudson's theorem".

KLM, UP, and symplectic camel

Consider now the covariance operator of $\widehat{\rho}$; it is defined as in classical statistical mechanics by

$$\Sigma_{\widehat{\rho}} = \begin{bmatrix} \mathrm{Cov}(X,X)_{\widehat{\rho}} & \mathrm{Cov}(X,P)_{\widehat{\rho}} \\ \mathrm{Cov}(P,X)_{\widehat{\rho}} & \mathrm{Cov}(P,P)_{\widehat{\rho}} \end{bmatrix}$$

where $\mathrm{Cov}(X,X)_{\widehat{\rho}} = (\mathrm{Cov}(X_j,X_k)_{\widehat{\rho}})_{1\leq j,k\leq n}$ with

$$\mathrm{Cov}(X_j,P_j)_{\widehat{\rho}} = \int_{\mathbb{R}^{2n}} (x_j - \langle x_j\rangle_{\widehat{\rho}})(x_k - \langle x_k\rangle_{\widehat{\rho}})\rho(z)dz$$

etc.... For instance, when $n = 1$:

$$\Sigma_{\widehat{\rho}} = \begin{bmatrix} (\Delta X)^2_{\widehat{\rho}} & \mathrm{Cov}(X,P)_{\widehat{\rho}} \\ \mathrm{Cov}(P,X)_{\widehat{\rho}} & (\Delta P)^2_{\widehat{\rho}} \end{bmatrix}.$$

Positivity and the KLM conditions

- It turns out that the KLM conditions ensuring positive semi-definiteness of $\widehat{\rho}$ imply (but are not equivalent to, except in the Gaussian case) the following condition on the condition $\Sigma_{\widehat{\rho}}$:

$$\Sigma_{\widehat{\rho}} + \frac{1}{2} i\hbar J \geq 0.$$

  This condition, well-known in quantum optics, is rigorously equivalent to the UP! But it is also equivalent to a topological condition, which can be stated in two equivalent ways. Consider the "Wigner ellipsoid" $W_{\widehat{\rho}} : \frac{1}{2}\Sigma_{\widehat{\rho}}^{-1} z \cdot z \leq 1$; then

- There is no way one can embed a phase space ball with radius $\sqrt{\hbar}$ into $W_{\widehat{\rho}}$ using only *canonical transformations* (but one can always find a general volume preserving transformations which does the job!).
- The symplectic capacity of the Wigner ellipsoid $W_{\widehat{\rho}}$ is $\geq \pi\hbar = \frac{1}{2}h$ (half the quantum of action...)

The Narcowich–Wigner Spectrum

- As we mentioned before, a given self-adjoint operator with trace one can be positive semi-definite for some values of Planck's constant, and not for others. The situation is particularly embarrassing when one wants to study the classical limit $\hbar \to 0$...

The Narcowich–Wigner Spectrum

- As we mentioned before, a given self-adjoint operator with trace one can be positive semi-definite for some values of Planck's constant, and not for others. The situation is particularly embarrassing when one wants to study the classical limit $\hbar \to 0$...
- Narcowich (1986) has introduced the notion of "Wigner spectrum". It is defined as follows: let ρ be such that $\int \rho(z)dz = 1$. Then $WS(\rho)$ is the set of all numbers $\eta \geq 0$ for which the KLM conditions are satisfied by ρ_σ: for *any* sequence $z_1, ..., z_N$ of phase space points $z_j = (x_j, p_j)$ the Hermitian $N \times N$ operator $M^\eta = (M^\eta_{jk})_{1 \leq j,k \leq N}$ with (j,k) entry

$$M^\eta_{jk} = \rho_\sigma(z_j - z_k)e^{-\frac{i}{2}\eta\sigma(z_j,z_k)}$$

is *positive-definite*.

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4. $WS(\rho) \subset [-A, A]$ for some $A \geq 0$.
5. $WS(\rho * \rho')$ contains $WS(\rho) + WS(\rho')$.

Two Questions...

- **Question 1:** For which quantum states $\widehat{\rho}$ do we have $WS(\rho) = [-\hbar, \hbar]$? This is an interesting question, because (if they exist) such states go "smoothly" to classical states when $\hbar \longrightarrow 0$.

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- **Question 2:** What about the condition $\{-\hbar, 0, \hbar\} \subset WS(\rho)$?

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- **Question 1:** For which quantum states $\widehat{\rho}$ do we have $WS(\rho) = [-\hbar, \hbar]$? This is an interesting question, because (if they exist) such states go "smoothly" to classical states when $\hbar \to 0$.
- **Question 2:** What about the condition $\{-\hbar, 0, \hbar\} \subset WS(\rho)$?

- **Answers**: Unknown in general.... Werner and Bröcker have shown that in general a mixture of the three first states of the harmonic oscillator does not satisfy $WS(\rho) = [-\hbar, \hbar]$, so such a mixture does not qualify for the limit $\hbar \to 0$. We can however give a characterization of pure states, following ideas of Narcowich, O'Connell, Dias, Prata....

Wigner Spectrum of Pure States

The following result completely describes the Wigner spectrum of the Wigner transform of a function in $L^2(\mathbb{R}^n)$:

Theorem

Let $\rho = W\psi$. Then:
(i) If ψ is (and hence ρ) a Gaussian then $WS(\rho) \supset [-\hbar, \hbar]$;
(ii) Otherwise $WS(\rho) = \{-\hbar, \hbar\}$.

Proof.

(i) Since the state is Gaussian we have $\eta \in WS(\rho)$ if and only if $\Sigma_{\widehat{\rho}} + \frac{1}{2}i\eta J \geq 0$. Since $\hbar \in WS(\rho)$ we have$\Sigma_{\widehat{\rho}} + \frac{1}{2}i\hbar J \geq 0$. Set now $\eta = r\hbar$ with $0 \leq r \leq 1$. We have

$$\Sigma_{\widehat{\rho}} + \frac{1}{2}i\eta J = (1-r)\Sigma_{\widehat{\rho}} + r\left(\Sigma_{\widehat{\rho}} + \frac{1}{2}i\hbar J\right) \geq 0.$$

□

Proof.

(ii) Set $G_\eta(z) = (\pi\eta)^{-n}\exp(-\frac{1}{\eta}|z|^2)$ for $\eta > 0$. Assume $WS(\rho)$ contains $\eta < \hbar$ (and > 0). We have

$$WS(G_\eta * \rho) \supset WS(G_\eta) + WS(\rho) \supset \{-\hbar, 0, \hbar\}$$

since $WS(G_\eta) = [-\eta, \eta]$ and $WS(\rho) \supset \{-\hbar, \eta, 0, \eta, \hbar\}$. It follows that $G_\eta * \rho$ is the Wigner distribution of some state; in view of the KLM conditions we also have $G_\eta * \rho \geq 0$. Define $F = G_\hbar * \rho$; we have $F \geq 0$ (it is a "Husimi distribution"). Since $G_\eta * G_{\eta'} = G_{\eta+\eta'}$ we can write $F = G_{\hbar-\eta} * (G_\eta * \rho)$ for $0 < \eta < \hbar$. But F is not a Gaussian (because ρ isn't) and hence there exists z_0 such that

$$F(z_0) = \int_{\mathbb{R}^n} e^{-\frac{1}{\hbar-\eta}|z_0-z|^2}(G_\eta * \rho)(z)dz = 0.$$

But this forces $G_\eta * \rho$ to be < 0 on a whole set with measure > 0, which is impossible because $G_\eta * \rho \geq 0$. □

Symplectic capacities

A symplectic capacity on the symplectic space $(\mathbb{R}^{2n}, \sigma)$ assigns to every subset Ω of $\mathbb{R}^{2n}$ a number $c(\Omega) \geq 0$ or $+\infty$; this assignment has the four properties listed below. We denote by $B(R)$ the ball $|z| \leq R$ and by $Z_j(R)$ the cylinder $x_j^2 + p_j^2 \leq R^2$.

- Monotonicity: $c(\Omega) \leq c(\Omega')$ if $\Omega \subset \Omega'$;
- Symplectic invariance: $c(f(\Omega)) = c(\Omega)$ *for every canonical transformation* f *(linear, or not);*
- Conformality: $c(\lambda\Omega) = \lambda^2 c(\Omega)$ *if* $\lambda \in \mathbb{R}$*;*
- Nontriviality: *We have* $c(B(R)) = c(Z_j(R)) = \pi R^2$.

Example

The "symplectic area" or "Gromov width"

$$c_{\mathrm{Gr}}(\Omega) = \sup_{f \text{ canonical}} \{\pi r^2 : f(B(R)) \subset \Omega\}.$$

That c_{Gr} is a symplectic capacity follows from Gromov's non-squeezing theorem (it is in fact equivalent to it).

Symplectic capacities and the UP

The Robertson–Schrödinger uncertainty principle

$$(\Delta X_j)^2_{\widehat{\rho}}(\Delta P_j)^2_{\widehat{\rho}} \geq [\mathrm{Cov}(X_j, P_j)_{\widehat{\rho}}]^2 + \tfrac{1}{4}\hbar^2$$

is equivalent to the condition

$$\Sigma_{\widehat{\rho}} + \frac{1}{2} i\hbar J \geq 0$$

which is equivalent to the condition

$$c(\mathcal{W}) \geq \pi\hbar = \frac{1}{2}h$$

for every symplectic capacity; here

$$\mathcal{W} : \frac{1}{2}\Sigma_{\widehat{\rho}}^{-1} z \cdot z \leq 1$$

is the so-called "Wigner ellipsoid".

Application: Sub-Gaussian Pure states

Let ψ be a normalized pure state (=wavefunction).

Theorem

Assume that there exists a real symmetric operator $M > 0$ *such that* $\rho(z) = W\psi(z) \leq Ce^{-\frac{1}{\hbar}Mz\cdot z}$.
(i) The ellipsoid $\mathcal{M} = \{z : Mz \cdot z \leq \hbar\}$ *has symplectic capacity* $c(\mathcal{M}) \geq \frac{1}{2}h$.
(ii) If $\mathcal{M}$ *is the image of the ball* $B(\sqrt{\hbar}) : |z|^2 \leq \hbar$ *by a linear symplectic transformation* S *then and* ψ *is a squeezed coherent state* $Ne^{-\frac{1}{2\hbar}(X+iY)x\cdot x}$, *image of* $\psi_0(x) = (\pi\hbar)^{-n/4}e^{-\frac{1}{2\hbar}|x|^2}$ *by any one of the two metaplectic operators corresponding to the symplectic operator* S;
(iii) In this case the Wigner spectrum of $\rho = W\psi$ *is* $[-\hbar, \hbar]$ *(and* $\lim_{\hbar\to 0}\rho(z) = \delta(z)$*).*

Sub-Gaussian Pure states

Proof.

(i) (Åskloster 2007!). The idea is to perform a symplectic diagonalization: $M = S^T DS$ and to use Hardy's uncertainty principle: Let ψ be square integrable and let $\widehat{\psi}(p)$ be its $\hbar$-Fourier transform. Assume that for some constant $C > 0$:

$$|\psi(x)| \leq Ce^{-\frac{a}{2\hbar}x^2} \text{ and } |\widehat{\psi}(p)| \leq Ce^{-\frac{b}{2\hbar}p^2}.$$

If $ab > 1$ then $\psi = 0$; If $ab = 1$ then $\psi(x) \sim e^{-\frac{a}{2\hbar}x^2}$. This leads to

$$W\psi(Sz) \leq C \exp\left[-\frac{1}{\hbar}\sum_{j=1}^{n}\lambda_j(x_j^2 + p_j^2)\right]$$

where $\lambda_1 \geq ... \geq \lambda_n$ are positive real numbers such that $\lambda_1 \leq 1$. The symplectic capacity of $\mathcal{M} = \{z : Mz \cdot z \leq \hbar\}$ is $c(\mathcal{M}) = \pi\hbar/\lambda_1 \geq \pi\hbar$. □

Sub-Gaussian Pure states

Proof.

(ii) We have $M = S^T S$ and $W\psi(Sz) \leq Ce^{-\frac{1}{\hbar}|z|^2}$. Since $W\psi(Sz) = W\widehat{S}^{-1}\psi(z)$ (symplectic/metaplectic covariance of the Wigner transform) Hardy's theorem now implies that we must have $\psi = \widehat{S}\psi_0$. (iii) is obvious. □

Sub-Gaussian Mixed states

Here is a generalization of the previous result:

Theorem

Assume that there exists a real symmetric operator $M > 0$ such that $\rho(z) \leq Ce^{-\frac{1}{\hbar}Mz\cdot z}$. If $\widehat{\rho}$ is a density operator then the ellipsoid $\mathcal{M} = \{z : Mz \cdot z \leq \hbar\}$ has symplectic capacity $c(\mathcal{M}) \geq \frac{1}{2}h$. (ii) If $\mathcal{M}$ is the image of the ball $B(\sqrt{\hbar}) : |z|^2 \leq \hbar$ by a linear symplectic transformation S then $c(\mathcal{M}) = \frac{1}{2}h$ has full Wigner spectrum: $WS(\rho) = [0, \hbar]$; in fact the state represented by $\widehat{\rho}$ is a pure (Gaussian) state.

Proof.

Using a symplectic diagonalization of M reduces the problem to the case where M is a diagonal operator; one then applies Hardy's uncertainty principle (cf. Åskloster 2007...) to show that M must satisfy the condition $M^{-1} + iJ \geq 0$, which is equivalent to $c(\mathcal{M}) \geq \frac{1}{2}h$. □

Here is a result that generalizes the Gaussian case:

Theorem

Let Q be a real C^2 function on $\mathbb{R}^n$ which is strictly and uniformly convex. Assume that there exists $C > 0$ such that $\rho(z) \leq Ce^{-\frac{1}{\hbar}Q(z)}$.
(i) If $\widehat{\rho}$ is a density operator then the set $\mathcal{C} = \{z : Q(z) \leq \hbar\}$ has symplectic capacity $c(\mathcal{C}) \geq \frac{1}{2}h$ for every symplectic capacity c;
(ii) equivalently $\oint_\gamma pdx \geq \frac{1}{2}h$ for every Hamiltonian periodic orbit γ carried by the boundary $\partial\mathcal{C}$.

Remark 1: Q is strictly and uniformly convex if and only if there exists $c > 0$ such that $Q''(z_0)z \cdot z \geq c|z|^2$ for all z_0, z. It follows that the set C is compact and convex.
Remark 2: Periodic Hamiltonian orbits on a hypersurface are defined unambiguously; such orbits always exist when $\partial\mathcal{C}$ bounds a convex and bounded set.

Sketch of Proof

1. We may assume $Q(0) = 0$ (trivial!) and $Q'(0) = \nabla_z Q(0) = 0$ (replace $\rho(z)$ by $\rho(z - z_0)$ for a suitably chosen z_0).

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2. The condition $Q''(z_0)z \cdot z \geq c|z|^2$ is equivalent to $\lambda_Q > 0$ where

$$\lambda_Q = \inf_{z \in \mathbb{R}^{2n}} \{\lambda(z) : \lambda(z) \textit{ is an eigenvalue of } Q''(z)\}.$$

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$$c(\mathcal{C}) \geq c(B(\sqrt{2\hbar/\lambda_Q})) \geq \tfrac{1}{2}h.$$

Sketch of Proof

5. That we have $c(\mathcal{C}) \geq \frac{1}{2}h \iff \oint_{\gamma_{\min}} pdx \geq \frac{1}{2}h$ in the Theorem follows from the existence of a particular symplectic capacity, the Hofer–Zehnder capacity c_{HZ}, which has the property that it is given by $c_{\mathrm{HZ}}(\Omega) = \oint_{\gamma_{\min}} pdx$ when Ω is a compact and convex set. (See H. Hofer and E. Zehnder. *Symplectic Invariants and Hamiltonian Dynamics*. Birkhäuser 1994.)

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THANK YOU!