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A ‘pointwise’ kinetic energy estimate and applications to Schrödinger theory

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Abstract. In this paper we provide a couple of estimates on eigenfunctions, eigenvalues, expectation values and the number of bound states in Schrödinger theory. Our main tool will be an almost ‘pointwise’ kinetic energy estimate which we prove to hold in all dimensions $n \geq 3$.

Introduction

In this paper we want to provide a couple of estimates on eigenvalues, eigenfunctions and the number of bound states of Schrödinger operators. Since this field has been widely and intensely studied in the last decade the mathematical methods have become rather advanced and complex. A relatively complete list of references can be found e.g. in the books of M. Reed and B. Simon (in particular [4], the review article in [5], for more special questions see also [6]) and the textbooks of W. Thirring ([7]).

A little bit in contrast to this we want to start in the following chapter from an energy estimate which will be derived by applying only rather elementary mathematics, more explicitly, we shall give an almost ‘pointwise’ lower bound of the kinetic energy by the wave function itself, which, despite of being rather natural, we have not found in the literature on partial differential equations.

This estimate turns out to be, owing to its ‘naturalness’, at the core of a couple of only loosely connected subjects in Schrödinger theory, which allows us to provide a unified approach to a class of problems which have been treated up to now by employing rather diverse methods. In particular, the approach does work in all dimensions $n \geq 3$, which is not merely academical having e.g. N -body Hamiltonians in mind. Furthermore, the momentum space analogue of the estimate yields bounds of the expectation of functions of the momentum operator resp. Laplacian by $\langle Q^2 \rangle$.

In the remaining sections of the paper we shall apply the results of Chapter 2 to several topics of Schrödinger theory. We shall e.g. treat selfadjointness questions and give lower bounds for Hamiltonians and eigenvalues in all dimensions $n \geq 3$ for various classes of potentials (in addition to the ‘usual’ atomic potentials we discuss also potentials with $V_- \equiv 0$ resp. $V(r) \rightarrow \infty$ for $r \rightarrow \infty$). The method allows furthermore to give simplified proofs for a couple of classical results of which we mention e.g. the one of Jost and Pais which we slightly extend to the case $E = 0$.

Along these lines one can also extend some of the classical estimates concerning the number of bound states n_l and the maximal angular momentum of eigenstates; i.e. we can show ($n = 3$):

$$n_l(V_-) \leq (1 - l(l+1)/Z) \cdot \int r V_- dr \quad \text{if} \quad Z := \sup_r r V_-(r) < \infty,$$

which is, taken the whole range of l values, stronger than e.g. the Bargmann bound since it approaches zero quadratically with l . These and related topics as well as an extension to N -body Hamiltonians will be discussed in more detail elsewhere.

2. 'Pointwise' lower bounds for $(\nabla\psi | \nabla\psi)$ and $(r \cdot \psi | r \cdot \psi)$

In this section we shall give an *a priori* estimate of the kinetic energy $\int \nabla\bar{\psi} \nabla\psi d^n x$ by $|\psi|^2$ itself, which is in some respect more sensitive than the usual lower bounds in terms of certain integrals over $|\psi|^2$. In the other direction it provides an estimate of the magnitude of the wavefunction by the kinetic energy. Furthermore, the result does apply to all dimensions $n \geq 3$; a special version holds also for $n = 1$. By performing the analogous manipulations in momentum space, we shall derive an *a priori* inequality in which the expectation value of r^2 bounds the expectation values of a large class of functions of the momentum.

Theorem 1. With ψ in the domain of definition $D_{-i\nabla}$ of $-i\nabla$ as an operator on $L^2(\mathbb{R}^n)$ we have:

(i) $\int_{|x|>r} \nabla\bar{\psi} \nabla\psi d^n x \geq (n-2)r^{(n-2)} \cdot m_\psi(r)$ for ψ element of \mathcal{S} and more generally

(ii) $\int \nabla\bar{\psi} \nabla\psi d^n x \geq \text{ess. sup}_r (n-2)r^{(n-2)} \cdot m_\psi(r)$ with $m_\psi(r) := \int |\psi(r, \Omega)|^2 d\Omega$, $d\Omega$ the Lebesgue measure on the unit sphere in n dimensions.

Remarks. There do exist a couple of related results in the literature concerning boundary value problems of part. diff. eq., running e.g. under the name 'restricting to submanifolds' (comp. [1] Chapter IV.9 or [8] Chapter I.5), and by which the L^2 -norm of functions on the boundary $\partial\Omega$ can be dominated by the Sobolev-norm W_2^1 in the interior Ω . However, at least as far as we can see, this would yield only a term r^{n-1} in contrast to r^{n-2} in our results which is too weak in this context. Furthermore the W_2^1 -norm contains a nasty non-derivative term which cannot be eliminated.

Proof. For all n , \mathcal{S} , the space of functions which decrease rapidly together with their derivatives is a domain of essential selfadjointness for $-i\nabla$ (with $D_{-i\nabla}$ defined by $\int |k|^2 |\hat{\psi}|^2(k) d^n k < \infty$, $\hat{\psi}$ the Fourier transformation of ψ). So we start with a $\psi \in \mathcal{S}(\mathbb{R}^n)$.

Choosing instead of x new coordinates $r := |x|$, Ω the coordinates on the unit sphere, we have for every x :

$$|\nabla\psi|^2(x) = \{|\nabla\psi|_r^2 + |\nabla\psi|_\Omega^2\}(x) \geq |\nabla\psi|_r^2(x) \quad (1)$$

where the indices r, Ω denote the projections of $\nabla\psi$ on the directions which span the local coordinate frame. Hence we get:

$$\int |\nabla\psi|^2 d^n x \geq \int |\nabla\psi|_r^2 d^n x = \int |\partial_r\psi|^2 d\Omega r^{n-1} dr \quad (2)$$

For Ω fixed we have:

$$\begin{aligned} |\psi(r, \Omega)|^2 &= \left| \int_r^\infty \partial_r\psi(r', \Omega) dr' \right|^2 = \left| \int_r^\infty \partial_r\psi(r', \Omega) r'^{(n-1/2)} \cdot r'^{-(n-1/2)} \cdot dr' \right|^2 \\ &\leq \int_r^\infty |\partial_r\psi|^2 r'^{(n-1)} dr' \cdot \int_r^\infty r'^{-(n-1)} dr' = (n-2)^{-1} r^{-(n-2)} \cdot \int_r^\infty |\partial_r\psi|^2 r'^{(n-1)} dr' \end{aligned} \quad (3)$$

and

$$\int_{|x|>r} |\nabla\psi|^2 d^n x \geq \int d\Omega \int_r^\infty |\partial_r\psi|^2 r'^{(n-1)} dr' \geq (n-2)r^{(n-2)} \cdot \int d\Omega |\psi(r, \Omega)|^2 \quad (4)$$

from which also $\int |\nabla\psi|^2 d^n x \geq \sup_r (n-2)r^{(n-2)} \cdot m_\psi(r)$ follows.

To derive this last result for all $\psi \in D_{-i\nabla}$ we need the following simple lemma:

Lemma 1. With $\psi \in L^2$, $\psi_k \rightarrow \psi$ in the L^2 -norm, the following holds:

$$s := \text{ess. sup.}_r \int |\psi|^2(r, \Omega) d\Omega \leq \lim_k \overline{s_k}$$

with $s_k := \text{ess. sup.}_r \int |\psi_k|^2(r, \Omega) d\Omega$.

Proof. By definition of the essential supremum there exists for all $\varepsilon > 0$ a set $\mathcal{O}_\varepsilon \subset \mathbb{R}$ with Lebesgue measure $\neq 0$ s.t. $\int |\psi|^2(r, \Omega) d\Omega > s - \varepsilon$ for $r \in \mathcal{O}_\varepsilon$. Let us assume the statement were wrong, i.e., that $s > \lim_k s_k$. With $\varepsilon := 1/2(s - \lim_k s_k)$ we get:

$$\begin{aligned} 0 &= \lim_k \int |\psi - \psi_k|^2 d^n x = \lim_k \int dr r^{n-1} \left(\int |\psi(r, \Omega) - \psi_k(r, \Omega)|^2 d\Omega \right) \\ &\geq \lim_k \int_{\mathcal{O}_\varepsilon} dr r^{n-1} (\cdot \cdot \cdot) \end{aligned} \quad (5)$$

The inequality $|a - b| \geq ||a| - |b||$ for normed spaces yields:

$$\int |\psi(r, \Omega) - \psi_k(r, \Omega)|^2 d\Omega \geq \left| \left(\int |\psi(r, \Omega)|^2 d\Omega \right)^{1/2} \right| - \left| \left(\int |\psi_k(r, \Omega)|^2 d\Omega \right)^{1/2} \right|^2$$

and with $\int |\psi(r, \Omega)|^2 d\Omega > \int |\psi_k(r, \Omega)|^2 d\Omega + \varepsilon/2$ for all $k > k_\varepsilon$, $r \in \mathcal{O}_\varepsilon$, which holds by the above definition of ε , we arrive at $\lim_k \int |\psi - \psi_k|^2 d^n x \neq 0$, that is, a contradiction. This implies that, for $\psi \in D_{-i\nabla}$ and $\psi_k \rightarrow \psi$, $\nabla\psi_k \rightarrow \nabla\psi$ in L^2 , $\psi_k \in \mathcal{S}$:

$$\begin{aligned} \int |\nabla\psi|^2 d^n x &= \lim_k \int |\nabla\psi_k|^2 d^n x = \lim_k \int |\nabla\psi_k|^2 d^n x \\ &\geq \lim_k \text{ess. sup.}_r (n-2)r^{n-2} \int |\psi_k(r, \Omega)|^2 d\Omega \geq \text{ess. sup.}_r (n-2)r^{n-2} m_\psi(r). \end{aligned} \quad (6)$$

The practical use of the result derived above lies mainly in the fact that a knowledge about $r^{(n-2)} \int |\psi|^2(r, \Omega) d\Omega$ gives direct access to bounds on expressions containing the potential V . In particular, the rhs of (6), which is in general only implicitly known, does not show up in the final expression of the results derived in the following chapter.

Before starting with the applications of our, up to now, technical result we want to give the momentum space analogue of Theorem 1 without providing the details of the proof. We get:

Theorem 2. (i) $(n-2) \operatorname{ess. \, supr.}_k |k|^{(n-2)} \cdot m_{\hat{\psi}}(|k|) \leq \int \nabla_k \hat{\psi} \nabla_k \hat{\psi} d^n k = (\psi | r^2 \psi)$ with $\psi \in D_{r^2}$.

(ii) For rotational symmetric F , that is in particular $F(-\Delta)$, $(\psi | r^2 \psi) \geq C_F |(\psi | F(-i\nabla)\psi)|$ holds with

$$C_F := (n-2) \left(\int_0^\infty |k| \cdot |F(|k|)| d|k| \right)^{-1} < \infty \quad (7)$$

being assumed and $\psi \in D_{r^2} \cap D_{F(-i\nabla)}$.

Proof. The proof of (i) is analogous to the proof of Theorem 1. As to (ii) we have with (i):

$$\begin{aligned} |(\psi | F(-i\nabla)\psi)| &= \left| \int |\hat{\psi}|^2(k) F(k) d^n k \right| \\ &\leq \operatorname{ess. \, supr.}_{|k|} |k|^{(n-2)} \cdot m_{\hat{\psi}}(|k|) \cdot \int_0^\infty |k| \cdot |F(|k|)| d|k| \\ &\leq (\psi | r^2 \psi) \cdot (n-2)^{-1} \cdot \int_0^\infty |k| \cdot |F(|k|)| d|k|. \end{aligned} \quad (8)$$

Remarks. This is in some sense a generalization of the uncertainty principle lemma to a large class of functions of momentum (which reads $(\psi | -\Delta\psi) > 1/4(\psi | r^{-2}\psi)$ from which the inverse statement follows at least heuristically, i.e., $(\psi | r^2\psi) > 1/4(\psi | (-\Delta)^{-1}\psi)$).

B. Simon kindly informed us that by using Hardy's inequality one can even prove that $r^{-1} \cdot p^{-2} \cdot r^{-1}$ is bounded (comp. e.g. [9]).

3. Lower bounds on eigenvalues and selfadjointness questions of Schrödinger operators

We split the potential V into $V_+ - V_-$ with the obvious meaning for V_\pm . For many questions only V_- is of relevance. Furthermore in many cases the potential becomes singular only in $x=0$, as e.g. in atomic physics. Another case of interest is where the potential goes to infinity for $|x| \rightarrow \infty$. We want to apply our inequality to these typical classes and compare it with the well-known uncertainty lemma approach (see e.g. [1], [2]).

To demonstrate how our inequality can be applied we discuss a typical problem of Schrödinger theory. With $H_0 := -\Delta$, $Q(H_0)$ the form domain of H_0 which is identical with $D(|-i\nabla|) = D(-i\nabla)$ (comp. [10], Chapter VI.2.6) we

assume V to be defined on $Q(H_0)$ in the form sense. If we have $|(\psi | V\psi)| \leq a(\psi | H_0\psi) + b(\psi | \psi)$ with $a < 1$ then we can define an operator H by means of the so called (KLMN) theorem (comp. [1] p. 167) with $Q(H) = Q(H_0)$ and $-b \leq (\psi | H\psi) = (\psi | H_0\psi) + (\psi | V\psi)$ on $Q(H_0)$ (since H and H_0 define equivalent graph norms on $Q(H_0)$).

Theorem 3. *Let V be rotational symmetric and defined on $Q(H_0)$ in the form sense. Furthermore we assume $rV(r) \in L^1(0, c)$ for some $c \geq n-2 \geq 1$ and that for all $\delta > 0$ $\sup_{r \geq \delta} |V|(r) < \infty$. Then we have:*

- (i) V is infinitesimally form bounded with resp. to H_0 .
- (ii) H is bounded from below by $-\sup_{r \geq r_{n-2}} |V|(r)$, (i.e. $\varepsilon = n-2$ below).

Proof. With $\psi \in Q(H_0)$ we have

$$\begin{aligned} |(\psi | V\psi)| &= \left| \int_0^\infty \left(\int |\psi(r, \Omega)|^2 d\Omega \right) \cdot V(r) r^{n-1} dr \right| \\ &\leq \int_0^{r_\varepsilon} |V|(r) r^{n-1} \cdot m_\psi(r) dr + \int_{r_\varepsilon}^\infty (\cdot \cdot \cdot) dr \end{aligned} \quad (9)$$

$$\leq \text{ess. sup.}_{r \leq r_\varepsilon} r^{n-2} \cdot m_\psi(r) \cdot \int_0^{r_\varepsilon} r |V|(r) dr + \sup_{r \geq r_\varepsilon} |V|(r) \cdot \|\psi\|^2 \quad (10)$$

where, according to our assumption, there exists for every $\varepsilon > 0$ a r_ε s.t. $\int_0^{r_\varepsilon} r |V| dr < \varepsilon$. With $(\psi | H_0\psi) \geq \text{ess. sup.}_{r \leq r_\varepsilon} (n-2)r^{n-2}m_\psi(r)$ we get:

$$|(\psi | V\psi)| \leq \varepsilon/n - 2(\psi | H_0\psi) + \sup_{r \geq r_\varepsilon} |V|(r) \cdot \|\psi\|^2; \quad \text{this proves (i).}$$

We have proved in addition that for $\varepsilon/n - 2 \leq 1$, $(\psi | H\psi) \geq -\sup_{r > r_\varepsilon} |V|(r)$, hence (ii).

Remarks. The condition imposed on V is natural; the border-line case is $|V| \sim r^{-2}$ in $r=0$, which is however not included. The relevant part of V will usually be V_- . We could have done the discussion with V_- instead of V and afterwards forming a s.a. operator H via the e.g. Friedrichs extension, (modulo certain domain questions).

While it is not intended here to give excellent lower bounds for the hamiltonian one should nevertheless remark that the lower bound of Theorem 3 is for the interesting potentials considerably better than the one derived from the uncert. princ. lemma; e.g. for potentials $-r^{-\alpha}$ and $n=3$ our bound is (i) $-(1/2-\alpha)^{\alpha/2-\alpha}$ in contrast to (ii) $-4^{\alpha/2-\alpha}$. For $\alpha=1$ this yields (i) -1 , (ii) -4 , with the exact lower bound $-1/4$ ($H = -\Delta - r^{-\alpha}$). For $\alpha=7/4$ the bounds become equal. In any case the bounds are easy to calculate.

Corollary 1. *For $V(x)$ not rotationally symmetric Theorem 3 does also apply if $|V|(r)$ is replaced by $|\bar{V}|(r) := \sup_\Omega |V|(r, \Omega)$.*

The above inequality can also be applied to Schrödinger operators in an electromagnetic field (A, Φ) . This problem is discussed e.g. in [1]. The hamiltonian reads:

$$H = (p - A)^2 + \Phi = -\Delta - 2iA \cdot \nabla - i(\nabla \cdot A) + A^2 + \Phi. \quad (11)$$

Performing the analogous splitting of the various parts of H as in Theorem 3 we can show that H is formbounded from below and that all terms of the interaction part are infinites. formbounded with resp. to $-\Delta$ provided that A_i can be split into a part lying in L^∞ and a contribution with a singularity at the origin $\leq r^{-1}$ which means roughly $A_i \in L^3 + L^\infty$. (For example for the sing. part, with $A_{\text{sing}} \equiv 0$ for $r > r_\varepsilon$:

$$\begin{aligned} |(\psi | A \cdot \nabla \psi)| &\leq (\psi | A^2 \psi)^{1/2} \cdot (\psi | -\Delta \psi)^{1/2} \quad \text{and} \quad (\psi | A^2 \psi)^{1/2} \\ &\leq \left(\int_0^{r_\varepsilon} r \cdot \left(\sup_{\Omega} A^2 \right) dr \right)^{1/2} \cdot (\text{ess. supr. } r^{(n-2)} \cdot m_\psi(r))^{1/2} \\ &\leq (\dots)^{1/2} \cdot (\psi | -\Delta \psi)^{1/2}; \quad \text{that is} \quad |(\psi | A \cdot \nabla \psi)| \leq \varepsilon' (\psi | -\Delta \psi). \end{aligned} \quad (12)$$

Another application is the following

Corollary 2. With $\int_0^\infty r \cdot |V|(r) dr$ resp. $\int_0^\infty r \cdot |\bar{V}|(r) dr < n-2$ $H = -\Delta + V$ is positive, i.e. $(\psi | H\psi) > 0$. That is, for a large class of potentials this excludes bound states ($E=0$ being included!).

Remarks. This is a classical result (for $n=3$!) derived by Jost and Pais ([3]) for eigenstates with $E < 0$ by using, however, completely different methods as e.g. convergence of the Born series; furthermore $E=0$ is automatically included in our approach.

We learned from B. Simon that in higher dimensions one can exploit dimensional relations (e.g. for $n, n-2$) between the various Beltrami operators in $\mathbb{R}^n, \mathbb{R}^{n-2}$ to lift results like these from e.g. $n=3$ to $n=5$, (as to the Beltrami operator for general n see e.g. [8]), provided one has already the Bargmann bound for $n=3$.

Proof. We have

$$\begin{aligned} |(\psi | V\psi)| &\leq \text{ess. supr.}_r r^{(n-2)} m_\psi(r) \cdot \int r \cdot |\bar{V}| dr \\ &\leq (n-2)^{-1} (\psi | -\Delta \psi) \cdot \int r \cdot |\bar{V}| dr \end{aligned} \quad (13)$$

and therefore $(\psi | (H_0 + V)\psi) \geq (\psi | -\Delta \psi) \cdot \{1 - (n-2)^{-1} \int r \cdot |\bar{V}| dr\}$. Since $\{\cdot \cdot \cdot\} > 0$ an eigenvalue $E=0$ would in particular imply $(\psi_0 | -\Delta \psi_0) = 0$, that is $\nabla \psi_0 = 0$ almost everywhere which is impossible for normalizable ψ_0 .

A further useful estimate can be accomplished by observing that there is nothing special about using $|\bar{V}|$ in the above calculations. In particular, for potentials going to $+\infty$ for $r \rightarrow \infty$, especially positive potentials, we can use another version to provide lower bounds.

Corollary 3. With $F(r)$ an arbitrary positive function s.t. $C_F := (n-2)^{-1} \int r \cdot F(r) dr < \infty$ and $(\psi | F\psi) < \infty$ on $Q(H_0)$ we have:

(i) $(\psi | -\Delta \psi) \geq C_F^{-1} \cdot (\psi | F(r)\psi)$ and

(ii) $(\psi | H\psi) \geq C_F^{-1} \cdot (\psi | F\psi) + (\psi | V\psi) \geq \inf_{r>0} \{C_F^{-1} \cdot F(r) + V(r)\} \|\psi\|^2$ with $Q(H) = Q(H_0)$.

Proof. The proof is obvious.

Remarks. (i) For many potentials where the other methods do not lead to sensible results (e.g. $V_- \equiv 0$, $V(0) = 0$ etc.) one can easily give lower bounds by choosing an appropriate $F(r)$ s.t. $F(r)$ is large where $V(r)$ is small resp. zero, thus making $\inf \{C_F^{-1} \cdot F(r) + V(r)\}$ as large as possible. A definite supremum is usually attained because C_F^{-1} becomes smaller when $F(r)$ grows.

(ii) To give a simple example where the exact lower bound is known take the harmonic oscillator for $n = 3$ ($H := -\Delta + r^2$). The exact lower bound is 3. With e.g. $F(r) := \sup \{-ar^2 + b, 0\}$, where $a, b > 0$, we get as a lower bound the value 2 for optimized a, b .

In the last section of this chapter we want to give an application to estimating all eigenvalues simultaneously. Sometimes one has the situation that the eigenvalues of the original hamiltonian $-\Delta + V_1$ can be computed while one is interested in the eigenvalues of $-\Delta + V_1 + \lambda V_2$.

Corollary 4. *Given a hamiltonian $H_\lambda := -\Delta + V_1 + \lambda V_2$ and $H^{(\varepsilon)} := -\varepsilon \Delta + V_1$, $0 < \varepsilon < 1$. We assume, for simplicity, that $Q(H_\lambda) = Q(-\Delta) = Q(H^{(\varepsilon)})$ for a certain λ -interval $[0, \lambda_0]$ and that $H^{(\varepsilon)}$ is bounded below; then we have:*

$$H_\lambda \geq -(1-\varepsilon)\Delta + V_1 \quad \text{for} \quad \lambda \leq \varepsilon(n-2) \cdot \left\{ \int r |\overline{V_2}| dr \right\}^{-1}, \quad \lambda \in [0, \lambda_0].$$

If $H^{(1-\varepsilon)}$, H_λ have eigenvalues $\{E_n(H_\lambda)\}$, $\{E_m(H^{(1-\varepsilon)})\}$ below the inf. of the ess. spectr., numbered from the bottom of the discrete spectrum, this implies $E_n(H_\lambda) \geq E_n(H^{(1-\varepsilon)})$ provided both H_λ , $H^{(1-\varepsilon)}$ have at least n eigenvalues.

Proof. We have

$$\begin{aligned} (\psi | -\Delta \psi) &= (1-\varepsilon)(\psi | -\Delta \psi) + \varepsilon(\psi | -\Delta \psi) \\ &\geq (1-\varepsilon)(\psi | -\Delta \psi) + \varepsilon(n-2) \left(\int r |\overline{V_2}| dr \right)^{-1} \cdot |(\psi | V_2 \psi)|, \end{aligned} \quad (14)$$

hence

$$\begin{aligned} (\psi | H_\lambda \psi) &\geq (1-\varepsilon) \cdot (\psi | -\Delta \psi) + (\psi | V_1 \psi) \\ &\quad + \left\{ \varepsilon(n-2) \left(\int r |\overline{V_2}| dr \right)^{-1} - \lambda \right\} |(\psi | V_2 \psi)|. \end{aligned}$$

That is, we can eliminate λV_2 for sufficiently small λ . The result for the eigenvalues follows from the min.max. principle (comp. e.g. [4]).

Remark. A typical case in point is e.g. the Coulomb problem with an additional perturbation.

4. Summary

We have given in this paper various applications of an a priori estimate of the kinetic energy which holds in all dimensions $n \geq 3$. While we have discussed

relatively abstract topics of Schrödinger theory we want to emphasize that the estimate can also be successfully applied to more concrete problems as e.g. estimating the l -dependent number of bound-states n_l in a central potential or the spreading of eigenfunctions as a function of l . These topics as well as applications to N -body hamiltonians shall be discussed elsewhere. As a last remark we want to mention that kinetic energy estimates are also of relevance in the realm of non linear part. diff. equations, hydrodynamics etc.

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