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ON THE LOCATION OF THE ESSENTIAL SPECTRUM OF SCHRÖDINGER OPERATORS

GIORGIO METAFUNE AND DIEGO PALLARA

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Abstract. We give estimates on the bottom of the essential spectrum of Schrödinger operators $-\Delta + V$ in $L^2(\mathbf{R}^N)$.

1. Introduction

In this note we give estimates on the bottom of the essential spectrum of Schrödinger operators $(A, D(A))$ in $\mathbf{R}^N$, where $A = -\Delta + V$ (Δ the usual Laplacian) and the potential $V : \mathbf{R}^N \to [0, \infty[$ is a positive, L^1_{loc}-function. We define A and its domain through the bilinear form

$$a(u, v) = \int_{\mathbf{R}^N} \big(\nabla u \cdot \nabla \bar{v} + V u \bar{v}\big),$$

defined for $u, v \in \mathcal{H} = \big\{u \in H^1(\mathbf{R}^N) : \int_{\mathbf{R}^N} V|u|^2 < \infty\big\}$. Hence,

$$\begin{aligned} &D(A) = \big\{u \in \mathcal{H} : \exists f \in L^2(\mathbf{R}^N) \text{ such that } a(u, v) = \textstyle\int_{\mathbf{R}^N} f\bar{v},\ \forall v \in \mathcal{H}\big\}, \\ &Au = f. \end{aligned} \tag{1.1}$$

The operator $(A, D(A))$ is self-adjoint and non-negative in $L^2(\mathbf{R}^N)$. If V is locally bounded, from local elliptic regularity the equality

$$D(A) = \big\{u \in \mathcal{H} \cap H^2_{\mathrm{loc}}(\mathbf{R}^N) : -\Delta u + V u \in L^2(\mathbf{R}^N)\big\}$$

follows. We recall that the discrete spectrum of a self-adjoint operator A consists of isolated eigenvalues of finite multiplicity; the remaining part of the spectrum is the essential spectrum, denoted by $\sigma_{\mathrm{ess}}(A)$. The resolvent of a self-adjoint operator A is compact if and only if $\sigma_{\mathrm{ess}}(A) = \emptyset$.

We prove lower estimates on the bottom of $\sigma_{\mathrm{ess}}(A)$ using a version of Poincaré inequality and measure-theoretic considerations. We denote by E_M the set $\{x \in \mathbf{R}^N : V(x) < M\}$, by $Q(c, d)$ an open cube of centre c and side d, and by $|E|$ the Lebesgue measure of E. Our arguments rely on the behaviour of the quantity

$$d^{-N} \left|E_M \cap Q(c, d)\right|,$$

as $|c| \to \infty$ and $Q(c, d)$ runs along a grid in $\mathbf{R}^N$ whose orientation is in some sense optimal. We used similar techniques in [8], where a characterisation of the

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compactness of the resolvent of A was given in the case of positive polynomial potentials, as conjectured by B. Simon in [10].

Upper and lower estimates of the bottom of $\sigma_{\rm ess}(A)$ are obtained in [7] (see also [6, Chapter 12]), using capacity methods as in Molcanov's characterization of the compactness of $(-\Delta+V)^{-1}$ for positive potentials V (see [9] or [3, Theorem VIII.4.1]). Similar arguments have been used in [5] to generalize Molcanov's criterion to some Riemannian manifolds. Taking into account the relation between capacity and Lebesgue measure, one can deduce from these results a lower estimate analogous to that in our Theorem 3.6. A more detailed comparison between the lower bounds obtained with these different approaches is done at the end of the paper. We point out that our methods cannot give upper bounds; on the other hand they are relatively elementary and yield explicit bounds.

If $x\in\mathbf{R}^N$ we set $|x|_\infty=\max_{i=1,\dots,N}|x_i|$. All integrals are understood with respect to the Lebesgue measure.

2. Poincaré inequality

In this section we collect some comments on Poincaré inequality in order to estimate the constants involved. Let us denote by $C(N,p)$ the best constant in Poincaré inequality in the unit cube $Q(1)$ (see e.g. [3, Th. V.3.24]):

$$\Big(\int_{Q(1)}|u-u_{Q(1)}|^p\Big)^{1/p}\le C(N,p)\Big(\int_{Q(1)}|\nabla u|^2\Big)^{1/2},\qquad u\in H^1(Q(1)),$$

where $u_{Q(1)}$ denotes the mean value of u in $Q(1)$. If $N=1$ the above estimate holds for every $1\le p\le\infty$, whereas for $N\ge 3$, $C(N,p)$ is defined for $1\le p\le 2^*=2N/(N-2)$ and $C(2,p)$ is defined for every $1\le p<\infty$. In all cases $C(N,p)$ is an increasing function of p so that $C(1,p)\le C(1,\infty)$, $C(N,p)\le C(N,2^*)$ for $N\ge 3$ and $C(2,p)\to+\infty$ as $p\to+\infty$.

An elementary Fourier series expansion shows that $C(1,\infty)=\sqrt{3}/3$. In fact, if $u\in H^1(0,1)$ satisfies $\int_0^1 u=0$, $\int_0^1|u'|^2=1$, then

$$u'(x)=\sum_{n\in\mathbf{Z}}a_ne^{2\pi inx}\quad\text{and}\quad u(x)=a_0\Big(x-\frac12\Big)+\sum_{n\ne0}\frac{a_n}{2\pi in}e^{2\pi inx}$$

with $\sum|a_n|^2=1$. Hence by Hölder's inequality

$$|u(x)|\le\frac{|a_0|}{2}+\frac{1}{2\sqrt3}\Big(\sum_{n\ne0}|a_n|^2\Big)^{1/2}=\frac{|a_0|}{2}+\frac{1}{2\sqrt3}\sqrt{1-|a_0|^2}.$$

The above function has maximum $\sqrt{3}/3$ in $[0,1]$ and this gives $C(1,\infty)\le\sqrt{3}/3$. The other inequality comes by taking $u(x)=x^2$.

A rescaling argument shows that for any $u\in H^1(Q(d))$

$$\Big(\int_{Q(d)}|u-u_{Q(d)}|^p\Big)^{1/p}\le C(N,p)d^{\frac{N}{p}+1-\frac{N}{2}}\Big(\int_{Q(d)}|\nabla u|^2\Big)^{1/2}. \tag{2.1}$$

If $N\ge3$ and $p=2^*$ the above inequality is scale-invariant; letting $d\to\infty$, one sees that $C(N,2^*)\ge S$, where S is the best constant in Sobolev's inequality

$$\Big(\int_{\mathbf{R}^N}|u|^{2^*}\Big)^{1/2^*}\le S\Big(\int_{\mathbf{R}^N}|\nabla u|^2\Big)^{1/2},\qquad u\in H^1(\mathbf{R}^N).$$

The exact value of S is computed in [12]. An upper bound for $C(N,2^*)$ can be obtained employing potential estimates as in [4, Chapter 7]. The inequality

$$|u(x)-u_{Q(1)}| \le N^{N/2-1} I_1(|\nabla u|)(x) := N^{N/2-1}\int_{Q(1)} \frac{|\nabla u(y)|}{|x-y|^{N-1}}\,dy \tag{2.2}$$

(see [4, Lemma 7.16]) and the boundedness of the Riesz potential $I_1 : L^2(Q(1)) \to L^{2^*}(Q(1))$ yield $C(N,2^*) \le N^{N/2-1}\|I_1\|$. Specializing the constants of [11, VIII, 4.2], one finally obtains

$$C(N,2^*) \le 2^{\frac{3}{2}-\frac{2}{N}} \cdot (3N)^{N/2}\Big(\frac{N\omega_N}{N-2}\Big)^{1-1/N},$$

where ω_N is the measure of the unit ball in $\mathbf{R}^N$. In order to estimate the growth of $C(2,p)$ as $p \to \infty$, we use inequality (2.2) and the boundedness of the Riesz potential $I_1 : L^2(Q(1)) \to L^p(Q(1))$ for every $p < \infty$ (see [4, Lemma 7.12], where the notation for I_1 is $V_{1/N}$). It turns out that

$$C(2,p) \le p^{1/p}\sqrt{\pi p} \le e^{1/e}\sqrt{\pi p} \tag{2.3}$$

for $2 \le p < \infty$.

Finally, notice that, estimating $|u_{Q(d)}|$ by Holder's inequality and using (2.1), it is easily seen that the following inequality holds for every $\varepsilon > 0$:

$$\begin{aligned} &\Big(\int_{Q(d)} |u|^p\Big)^{2/p} \\ &\le d^{\frac{2N}{p}-N}\Big[C^2(N,p)d^2\Big(1+\frac{1}{\varepsilon}\Big)\int_{Q(d)}|\nabla u|^2 + (1+\varepsilon)\int_{Q(d)}|u|^2\Big]. \end{aligned} \tag{2.4}$$

Estimates of the above type, i.e.,

$$\Big(\int_{Q(1)} |u|^p\Big)^{2/p} \le A\int_{Q(1)}|\nabla u|^2 + B\int_{Q(1)}|u|^2$$

are widely studied, even with the aim of finding the optimal constant A for a fixed B and vice versa. In order to obtain the best estimates on the essential spectrum with our method, our interest is to take B as close to 1 as possible (obviously, B cannot be smaller than 1). The above argument gives an estimate of the corresponding constant A, but we do not know its optimal value.

3. Estimates for the essential spectrum

We denote by Γ_d the set of all the grids γ in $\mathbf{R}^N$ whose elements are pairwise disjoint open cubes of side d such that $\bigcup_{Q\in\gamma}\overline{Q} = \mathbf{R}^N$. For every $M > 0$ define

$$\alpha_{d,M} := \inf_{\gamma\in\Gamma_d}\limsup_{\substack{|c|\to\infty\\ Q(c,d)\in\gamma}} \frac{|E_M \cap Q(c,d)|}{d^N}.$$

Theorem 3.1. *Let $N \ge 3$, let $C = C(N,2^*)$ be the constant in (2.1) for $p = 2^*$ and let $d > 0$. Assume that $\alpha_{d,M} \le \alpha < 1$ for every $M > 0$. Then*

$$\sigma_{\rm ess}(A) \subset \Big[\frac{(1-\alpha^{1/N})^2}{C^2 d^2 \alpha^{2/N}}, \infty\Big[.$$

Proof. Fix $\eta > 0$ and $\beta \in]\alpha, 1[$, and let $R > 0$ be such that for $M = \eta^{-1}$ the implication

$$|c|_\infty > R \qquad \Longrightarrow \qquad |E_M \cap Q(c,d)| \le \beta d^N$$

holds for some grid; without loss of generality we may suppose that the cubes of this grid have sides parallel to the axes. Henceforth, we assume $|c|_\infty > R$. Then

$$\int_{Q(c,d)\setminus E_M} |u|^2 \le \eta \int_{Q(c,d)\setminus E_M} V|u|^2 \le \eta \int_{Q(c,d)} V|u|^2. \tag{3.1}$$

By Hölder's inequality we have for $2 < p \le 2^*$

$$\int_{Q(c,d)\cap E_M} |u|^2 \le |E_M \cap Q(c,d)|^{1-2/p} \Big(\int_{Q(c,d)\cap E_M)} |u|^p \Big)^{2/p}. \tag{3.2}$$

Using (2.4) we obtain, writing $C(p)$ instead of $C(N,p)$,

$$\begin{aligned} &\int_{Q(c,d)\cap E_M} |u|^2 \\ &\le \beta^{1-2/p} \Big[C^2(p) d^2 \Big(1 + \frac{1}{\varepsilon}\Big) \int_{Q(c,d)} |\nabla u|^2 + (1+\varepsilon) \int_{Q(c,d)} |u|^2 \Big]. \end{aligned} \tag{3.3}$$

From (3.1) and (3.3), summing over a partition of $\{|x|_\infty \ge R\}$ in cubes of side d, we deduce

$$\begin{aligned} &\int_{\{|x|_\infty \ge R\}} |u|^2 \\ &\le \int_{\{|x|_\infty \ge R\}} \Big\{ \eta V|u|^2 + \beta^{1-2/p} \left[C^2(p) d^2 (1 + 1/\varepsilon) |\nabla u|^2 + (1+\varepsilon)|u|^2 \right] \Big\}. \end{aligned} \tag{3.4}$$

Choosing ε in (3.4) such that $\beta^{1-2/p}(1+\varepsilon) < 1$ and defining the following perturbed potential

$$\tilde V(x) = \begin{cases} \dfrac{1 - \beta^{1-2/p}(1+\varepsilon)}{\eta} & \text{if } \ |x|_\infty < R \text{ and } V(x) < \dfrac{1 - \beta^{1-2/p}(1+\varepsilon)}{\eta}, \\ V(x) & \text{otherwise,} \end{cases}$$

we obtain the inequality

$$\begin{aligned} &\frac{1 - \beta^{1-2/p}(1+\varepsilon)}{\beta^{1-2/p} d^2 C^2(p)(1+1/\varepsilon)} \int_{\mathbf{R}^N} |u|^2 \\ &\le \int_{\mathbf{R}^N} |\nabla u|^2 + \frac{\eta}{\beta^{1-2/p} d^2 C^2(p)(1+1/\varepsilon)} \int_{\mathbf{R}^N} \tilde V |u|^2. \end{aligned}$$

Setting

$$V_\eta = \frac{\eta}{\beta^{1-2/p} d^2 C^2(p)(1+1/\varepsilon)} V, \qquad \tilde V_\eta = \frac{\eta}{\beta^{1-2/p} d^2 C^2(p)(1+1/\varepsilon)} \tilde V,$$

we infer that

$$-\Delta + \tilde V_\eta \ge \frac{1 - \beta^{1-2/p}(1+\varepsilon)}{\beta^{1-2/p} d^2 C^2(p)(1+1/\varepsilon)} I$$

and hence that

$$\sigma_{\text{ess}}(-\Delta+\tilde{V}_\eta)\subset\Big[\frac{1-\beta^{1-2/p}(1+\varepsilon)}{\beta^{1-2/p}d^2C^2(p)(1+1/\varepsilon)},\infty\Big[.$$

Since $V_\eta-\tilde{V}_\eta$ is bounded with compact support, by [1, Lemma 1.6.5] we deduce that for λ large enough the operator $(-\Delta+V_\eta+\lambda)^{-1}-(-\Delta+\tilde{V}_\eta+\lambda)^{-1}$ is compact and then an application of [2, Theorem 8.4.3] gives $\sigma_{\text{ess}}(-\Delta+V_\eta)=\sigma_{\text{ess}}(-\Delta+\tilde{V}_\eta)$. Choosing $\eta=\beta^{1-2/p}d^2C^2(p)(1+1/\varepsilon)$ so that $V_\eta=V$ we obtain

$$\sigma_{\text{ess}}(-\Delta+V)\subset\Big[\frac{1-\beta^{1-2/p}(1+\varepsilon)}{\beta^{1-2/p}d^2C^2(p)(1+1/\varepsilon)},\infty\Big[$$

for every $\beta\in]\alpha,1[$, $\varepsilon>0$ such that $\beta^{1-2/p}(1+\varepsilon)<1$. The maximum of the function

$$\frac{1-t(1+\varepsilon)}{t(1+1/\varepsilon)}$$

in the range $\alpha^{1-2/p}\le t\le 1$, $t(1+\varepsilon)\le 1$ is $(1-\alpha^{1/p-1/2})^2$, hence we obtain that

$$\sigma_{\text{ess}}(A)\subset\Big[\frac{(\alpha^{1/p-1/2}-1)^2}{C^2(p)d^2},\infty\Big[.$$

Taking $p=2^*$, the thesis is proved. □

If $N=1$ we can use (3.3) for any p; letting $p\to\infty$ and recalling that $C(1,\infty)=\sqrt{3}/3$, we can argue as in the above theorem and deduce the following result.

Theorem 3.2. *Suppose that $N=1$ and that for some $d>0$ the upper bound $\alpha_{d,M}\le\alpha<1$ holds for any $M>0$. Then $\sigma_{\text{ess}}(A)\subset\Big[\frac{3(1-\sqrt{\alpha})^2}{d^2\alpha},\infty\Big[$.*

We consider now the case $N=2$. In view of the discussion in Section 2 about the behaviour of $C(2,p)$, we cannot expect an estimate as explicit as in the other cases.

Theorem 3.3. *Suppose that $N=2$ and that for some $d>0$ the upper bound $\alpha_{d,M}\le\alpha<1$ holds for any $M>0$. Then*

$$\sigma_{\text{ess}}(A)\subset\Big[\frac{e^{r(\alpha)/2}-\sqrt{\alpha}}{2e^{1/e}\pi}\cdot\frac{1}{d^2\alpha\log|\alpha|},\infty\Big[,$$

where $r(\alpha)\to 1$ as $\alpha\to 0$.

Proof. As in the proof of Theorem 3.1 we obtain that the infimum of $\sigma_{\text{ess}}(A)$ is greater than or equal to $\frac{(\alpha^{1/p-1/2}-1)^2}{C^2(2,p)d^2}$ for every $2\le p<\infty$. Estimate (2.3) implies that

$$\frac{(\alpha^{1/p-1/2}-1)^2}{C^2(2,p)d^2}\ge\frac{(\alpha^{1/p-1/2}-1)^2}{d^2e^{2/e}\pi p}.$$

The maximum of the function $p^{-1}(\alpha^{1/p-1/2}-1)^2$ for $2\le p<\infty$ is achieved at a point $p(\alpha)=(2|\log\alpha|)/r(\alpha)$ with $r(\alpha)$ as in the statement. This completes the proof. □

Remark 3.4. The condition $\alpha_{d,M}\le\alpha<1$ does not change if a constant is added to V. Hence the above theorems are particularly significant if $\liminf_{|x|\to\infty}V(x)=0$; in the general case they can be applied to the modified potential $V(x)-\liminf\limits_{|x|\to\infty}V(x)$.

From the preceding results we can generalise Theorem 3.1 in [8] (see also [5, Corollary 6.2]).

Corollary 3.5. *If for some $d > 0$ we have $\alpha_{d,M} = 0$ for every M or $\alpha_{d,M} \le \alpha < 1$ for arbitrary $d > 0$, then $\sigma_{\mathrm{ess}}(-\Delta + V) = \emptyset$, i.e., A has compact resolvent.*

Another estimate on the bottom of the essential spectrum of $(A, D(A))$ can be obtained, with similar methods, assuming an upper bound on $\alpha_{d,M}$ with M fixed and arbitrary $d > 0$.

Theorem 3.6. *Let $M > 0$ and assume that $\alpha_{d,M} \le \alpha < 1$ holds for every $d > 0$. Then $\sigma_{\mathrm{ess}}(A) \subset [M(1-\alpha^{2/N}), \infty[$ if $N \ge 3$ and $\sigma_{\mathrm{ess}}(A) \subset [M(1-\alpha), \infty[$ if $N = 1, 2$.*

Proof. Let $\alpha < \beta < 1$, $p = 2^*$ if $N \ge 3$ or $2 < p < \infty$ if $N = 1, 2$. Choose $\varepsilon > 0$ such that $\beta^{1-2/p}(1+\varepsilon) < 1$. Arguing as in the proof of Theorem 3.1, with $C(p) = C(N, p)$, one finds for every $d > 0$ a constant $R > 0$ such that

$$\begin{aligned} &M\big(1 - \beta^{1-2/p}(1+\varepsilon)\big) \int_{\{|x|_\infty \ge R\}} |u|^2 \\ &\le \int_{\{|x|_\infty \ge R\}} \Big\{ V|u|^2 + MC^2(p) d^2 \beta^{1-2/p}(1+\varepsilon) |\nabla u|^2 \Big\}. \end{aligned}$$

The inequality

$$M\big(1 - \beta^{1-2/p}(1+\varepsilon)\big) \int_{\{|x|_\infty \ge R\}} |u|^2 \le \int_{\{|x|_\infty \ge R\}} \big(V|u|^2 + |\nabla u|^2\big)$$

then follows choosing d such that $MC^2(p) d^2 \beta^{1-2/p}(1+\varepsilon) \le 1$ and implies that the essential spectrum of A is contained in $[M\big(1 - \beta^{1-2/p}(1+\varepsilon)\big), \infty[$. Letting $\beta \to \alpha$, $\varepsilon \to 0$ and $p \to \infty$ if $N = 1, 2$, the thesis follows. □

Since A is self-adjoint and non-negative, it generates a strongly continuous semigroup of self-adjoint operators e^{-tA}. From the preceding results the exponential stability of e^{-tA} can easily be deduced.

Corollary 3.7. *Under the hypotheses of one of the above theorems, there exists a positive δ such that $\|e^{-tA}\| \le e^{-\delta t}$, $t \ge 0$.*

Proof. It is sufficient to show that $\sigma(A) \subset [\delta, \infty[$ for some positive δ. To this aim we observe that each of Theorems 3.1, 3.2, 3.3 and 3.6 implies that $\sigma_{\mathrm{ess}}(A) \subset [\delta_1, \infty[$ for some $\delta_1 > 0$. Moreover, 0 is not an eigenvalue of A; in fact the identity

$$\int_{\mathbf{R}^N} \big(V|u|^2 + |\nabla u|^2\big) = 0$$

yields $u \equiv 0$, because $V \ge 0$. It follows that 0 belongs to the resolvent set and hence $\sigma(A) \subset [\delta, \infty[$ for some positive δ. □

We end with a comparison of our results and those of [7]. While we do not see any connection between [7] and our Theorem 3.1, it is interesting to point out some relations with our Theorem 3.6. The results of Maz'ya and Otelbaev cover more general cases; in fact, elliptic operators of higher order and non-absolutely continuous potentials V are allowed. These authors use capacity methods and obtain two-side estimates on the bottom Γ of $\sigma_{\mathrm{ess}}(A)$. On the other hand, we start from measure-theoretic estimates and this leads only to lower bounds for Γ.

Taking into account the following relation between the measure and the capacity of a compact set $E \subset \Omega \subset \mathbf{R}^N$ (see [6, Sect. 2.2.3])

$$\mathrm{cap}_\Omega(E) \geq c_1(N)|E|^{(N-2)/N} \quad (N \geq 3)$$

we may compare the lower bound of [7] with that of our Theorem 3.6, confining ourselves to the case $N \geq 3$. We refer to [6] for the properties of capacities.

A compact set $E \subset Q(c,d)$ is inessential in $Q(c,d)$ if its capacity with respect to the cube $Q(c,2d)$ is smaller than γd^{N-2} where γ is a constant depending only on the dimension N. Let $N(Q(c,d))$ be the family of all inessential subsets of $Q(c,d)$ and define

$$D_R = \sup\Big\{d : \exists Q(c,d) \text{ with } |c|_\infty \geq R \text{ and } \inf_{E \in N(Q(c,d))} \int_{Q(c,d)\setminus E} V(x)\,dx \leq d^{N-2}\Big\},$$

and $D_\infty = \lim_{R\to\infty} D_R$. In [7] the estimate $\Gamma \geq c_2 D_\infty^{-2}$ is proved, with c_2 depending only on N.

Setting $\alpha_0 = (\gamma/c_1)^{N/(N-2)}$, assume that there is $M > 0$ such that

$$\limsup_{|c|\to\infty} \frac{|E_M \cap Q(c,d)|}{d^N} < \alpha_0$$

for all $d > 0$. Since

$$\begin{aligned}
&\inf_{E \in N(Q(c,d))} \int_{Q(c,d)\setminus E} V(x)\,dx \geq \inf\Big\{\int_{Q(c,d)\setminus E} V(x)\,dx : |E \cap Q(c,d)| \leq \alpha_0 d^N\Big\} \\
&= \inf\Big\{\int_{Q(c,d)\setminus E} V(x)\,dx : E \supset E_M \text{ and } |E \cap Q(c,d)| \leq \alpha_0 d^N\Big\} \\
&\geq M|Q(c,d) \setminus E_M|,
\end{aligned}$$

for every cube $Q(c,d)$, we easily deduce that $D_\infty \leq [M(1-\alpha_0)]^{-1/2}$. This gives $\Gamma \geq c_2 M(1-\alpha_0)$, and hence a dependence on M similar to that in Theorem 3.6. Observe however that Theorem 3.6 also gives a dependence of Γ on α on the whole interval $[0,1]$.

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Dipartimento di Matematica "Ennio De Giorgi", Università di Lecce, C.P.193, 73100, Lecce, Italy
E-mail address: metafune@le.infn.it

Dipartimento di Matematica "Ennio De Giorgi", Università di Lecce, C.P.193, 73100, Lecce, Italy
E-mail address: pallara@le.infn.it