# Nonrelativistic Hydrogen type stability problems on nonparabolic 3-manifolds

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Güneysu, B.: *Nonrelativistic Hydrogen type stability problems on nonparabolic 3-manifolds*. Ann. Henri Poincaré (2012).

Partially:

Güneysu, B.: *On generalized Schrödinger semigroups.* J. Funct. Anal. 262 (2012), 4639–4674.

Güneysu, B. & Post, O.: *Path integrals and the essential self-adjointness of differential operator on noncompact manifolds*. Preprint (2012), arxiv.

Güneysu, B.: *Kato's inequality and form boundedness of Kato potentials on arbitrary Riemannian manifolds.* Proc. Amer. Math. Soc. (2012).

# Review of the Euclidean $\mathbb{R}^3$

- $\kappa \geq 0$, $y \in \mathbb{R}^3$, $\beta \in \Omega^1_{\mathbb{R}}(\mathbb{R}^3)$ and $G(x,y) = 1/|x-y|$
- Under $\int_{\mathbb{R}^3} |\mathrm{d}\beta|^2 \,\mathrm{d}x < \infty$, there is a unique self-adjoint realization $H(\beta, y, \kappa)$ of $\frac{1}{2}\left(\sum_j \sigma^j(\partial_j + \mathrm{i}\beta_j)\mathbf{1}\right)^2 - \kappa G(\bullet, y)\mathbf{1}$ in $\mathrm{L}^2(\mathbb{R}^3, \mathbb{C}^2)$
$\rightarrow$ Nonr. Hamilton operator of an atom with one electron (spin!) and a nucleus (fixed in $y$) with $\sim \kappa$ protons, in magnetic field $\mathrm{d}\beta$
- Classic result (Fröhlich/Lieb/Loss, 1986):
There are $C, \kappa_0 > 0$ such that for all $0 \leq \kappa \leq \kappa_0$ and all $\beta$, $y$ as above one has

$$H(\beta, y, \kappa) + \frac{1}{8\pi}\int_{\mathbb{R}^3} |\mathrm{d}\beta|^2 \,\mathrm{d}x \geq -C\kappa^2$$

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# Problem

Which topological and Riemann geometric properties of the Euclidean $\mathbb{R}^3$ guarantee the formulation and the proof of this stability problem?

$M$: Riemannian 3-manifold, with

$\mathrm{vol}(\mathrm{d}x)$: Riemannian volume measure

$\Delta = -\mathrm{d}^{\dagger}\mathrm{d}$: Laplace-Beltrami operator

$p_t(x, y)$: minimal positive heat kernel

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# Nonparabolicity I

## Definition

a) $\tilde{G}: M \times M \to [-\infty, \infty]$ is called a *Green's function* on $M$, if $\tilde{G}(x,y) = \tilde{G}(y,x)$, $\tilde{G}(x,\bullet) \in \mathrm{L}^1_{\mathrm{loc}}(M)$ and

$$-\Delta \tilde{G}(x,\bullet) = \delta_x \quad \text{for all } x, y \in M.$$

b) $M$ is called *nonparabolic*, if there is a positive Green's function on $M$.

- Green's functions exist on $M$, if and only if $M$ is noncompact
- $M$ is nonparabolic $\Leftrightarrow$ Brownian motions on $M$ are transient $\Leftrightarrow \int_0^\infty p_t(x,y)\mathrm{d}t < \infty$ for some/all $x \neq y$. Then $G(x,y) := \int_0^\infty p_t(x,y)\mathrm{d}t$ is the *minimal positive* Green's function on $M$
  $\to$ $G$ is our *Coulomb potential* !

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# Nonparabolicity II

**Theorem (ess. Varopoulos 1985; B.G.)**

*Let $M$ be complete and assume that there is $C_1 > 0$ such that for all $t > 0$, $x \in M$ one has the Gauss type upper bound*

$$p_t(x,x) \leq C_1 t^{-\frac{3}{2}} \qquad (\mathscr{G}).$$

*a) $M$ is nonparabolic and one has $G(\bullet, y) \in \mathcal{K}(M)$ for all $y \in M$, with $\mathcal{K}(M)$ the probabilistic Kato class of $M$.*
*b) There is a $C_2 > 0$ such that for any $h \in \mathrm{H}^{1,2}(M)$ one has*

$$\left(\int_M |h|^6 \,\mathrm{dvol}\right)^{\frac{1}{3}} \leq C_2 \int_M \left|\nabla^{\mathrm{T}M} h\right|^2 \mathrm{dvol} \quad (\mathscr{S})$$

$\rightarrow$ Geometric conditions for validity of $(\mathscr{G})$ are well-known

# Pauli-Dirac structures

- A *Pauli-Dirac structure* on the Riemannian manifold $M$ is a rank-2-Dirac structure $(c, \nabla)$ on $M$, that is, $c$ is a Clifford multiplication, $\nabla$ is a Clifford connection, and these date live on a complex Hermitian vector bundle over $M$ with fiber dimension 2
  $\to \mathscr{P}(c, \nabla) := \mathscr{D}(c, \nabla)^2$ is our *Pauli operator*
- The Riemannian manifold $M$ admits Pauli-Dirac structures, if and only if the topological manifold $M$ is $\mathrm{spin}^{\mathbb{C}}$
- If $(c, \nabla)$ is a Pauli-Dirac structure on $M$, then $\mathrm{tr}[\nabla^2]/\mathrm{i} \in \Omega^2(M)$ is a magnetic field and

$$\mathscr{P}(c, \nabla) = \nabla^{\dagger}\nabla + \frac{1}{4}\mathrm{scal}(\bullet)\mathbf{1} + \frac{1}{2}\sum_{i<j} \mathrm{tr}\left[\nabla^2\right](e_i, e_j)c(e_i^*)c(e_j^*)$$

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# The Hamiltonians under consideration I: Definition

We set

$$V[c,\nabla] := \frac{1}{4}\mathrm{scal}(\bullet)\mathbf{1} + \frac{1}{2}\sum_{i<j} \mathrm{tr}\left[\nabla^2\right](e_i,e_j)c(e_i^*)c(e_j^*)$$

$$S[c,\nabla] := \int_M \Big|V[c,\nabla]\Big|^2_{\mathrm{HS}} \mathrm{dvol}.$$

In $\mathbb{R}^3$, $S[c,\nabla]$ is just the magnetic energy!

**Theorem (B.G.; also B.G. & O. Post )**

*Let $M$ be complete with $(\mathscr{G})$. Then for any Pauli-Dirac structure $(c,\nabla)$ on $M$ with $S[c,\nabla]<\infty$ and any $y\in M$, the operator $\mathscr{P}-\kappa G(\bullet,y)\mathbf{1}$ is essentially self-adjoint on smooth compactly supported sections. The closure $H(c,\nabla;\kappa,y)$ is bounded from below.*

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# The Hamiltonians under consideration II: Path integrals

## Theorem (B.G.)

*Let $M$ be complete with $(\mathscr{G})$. Then*

$$\mathrm{e}^{-tH(\dots;\kappa,y)}f(x) = \mathbb{E}\left[\mathrm{e}^{\kappa\int_0^t G(B_s(x),y)\mathrm{d}s}\mathscr{V}_t^x //_t^{x,-1} f(B_t(x)) 1_{\{t<\zeta_x\}}\right],$$

*where*

- $B(x)$ *is a Brownian motion on* $M$ *with lifetime* $\zeta_x$,
- $//^x$ *is the stochastic parallel transport along* $B(x)$,
- $\mathscr{V}^x$ *is the unique (pathwise weak) solution of*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{V}_t^x = -\mathscr{V}_t^x //_t^{x,-1} V(B_t(x)) //_t^x,\ \mathscr{V}_0^x = \mathbf{1}.$$

$\to$ leads to $L^2 \to L^p$ bounds, smoothing properties, etc.

# The stabilty result

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*Let $M$ be complete with $(\mathscr{G})$. Then there are constants $C, \kappa_0 > 0$ such that for all Pauli-Dirac structures $(c, \nabla)$ on $M$ with $S[c, \nabla] < \infty$ and all $\Lambda > 0$, $0 \leq \kappa \leq \kappa_0 \Lambda^2$, $y \in M$ one has*

$$H(c, \nabla; \kappa, y) + \Lambda S[c, \nabla] \geq -C\kappa^2.$$

- Proof uses Kato property of $G(\bullet, y)$ (for uniformity in $y$), generalized Kato's inequality (for uniformity in $\nabla$) and $(\mathscr{S})$ (for uniformity in $V[c, \nabla]$) $\to$ We only use Dirichlet space methods (so no curvature estimates etc.) !
- The better the constants in $(\mathscr{G})$ and $(\mathscr{S})$ are, the bigger becomes $\kappa_0$
- Open: Multi-particle case under $(\mathscr{G})$ (essentially $\Leftrightarrow$ electrostatic inequality for $G(x, y)$)

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