ESI **The Erwin Schrödinger International Institute for Mathematical Physics**

Boltzmanngasse 9
A-1090 Wien, Austria

Regularity of the nodal sets of solutions to Schrödinger equations

M. Hoffmann-Ostenhof
T. Hoffmann-Ostenhof
N. Nadirashvili

Vienna, Preprint ESI 36 (1993) July 9, 1993

Supported by Federal Ministry of Science and Research, Austria

REGULARITY OF THE NODAL SETS OF SOLUTIONS TO SCHRÖDINGER EQUATIONS

M. Hoffmann-Ostenhof[1]
T. Hoffmann-Ostenhof[2,3]
N. Nadirashvili[3]

Institut für Mathematik, Universität Wien[1]
Institut für Theoretische Chemie, Universität Wien[2]
International Erwin Schrödinger Institute for Mathematical Physics[3]

1. Introduction

Let Ω be an open set in $\mathbb{R}^n$ and let $V : \Omega \to \mathbb{R}$ be real valued with $V \in L^1_{\text{loc}}(\Omega)$. We consider real valued solutions $u \neq 0$ which satisfy

$$\Delta u = Vu \text{ in } \Omega \tag{1.1}$$

in the distributional sense.

In a recent paper two of us [HO2] investigated the local behaviour of such solutions under rather mild assumptions on the potential V, namely we assumed that $V \in K^{n,\delta}(\Omega)$ for some $\delta > 0$, see e.g. [AS,S], where the class $K^{n,\delta}$ is defined by requiring that

$$\lim_{\varepsilon \downarrow 0} \sup_{x \in \mathbb{R}^n} \int_{|x-y|<\varepsilon} \chi_\Omega \frac{|V(y)|}{|x-y|^{n-2+\delta}} dy = 0 \tag{1.2}$$

Here χ_Ω denotes the characteristic function of Ω.

One of our main results was

Theorem 1.1. *Suppose $u \neq 0$ is a real valued solution of* (1.1). *Let $x_0 \in \Omega$ then either there is a harmonic homogenous polynomial $P_M \neq 0$ of degree M such that*

$$u(x) = P_M(x - x_0) + \Phi(x) \tag{1.3}$$

with

$$\Phi(x) = O(|x - x_0|^{M+min(1,\delta')}) \quad \forall \delta' < \delta \quad \textit{for } x \to x_0 \tag{1.4}$$

or u vanishes at x_0 faster than polynomially, that is

$$\overline{\lim_{x \to x_0}} |x - x_0|^{-\alpha} |u(x)| = 0$$

Typeset by $\mathcal{AMS}$-TEX

Typeset by $\mathcal{AMS}$-TEX

for every $\alpha > 0$.

It is known [AS,S] that $V \in K^{n,\delta}(\Omega)$, $\delta < 1$ implies $u \in C^{0,\delta}(\Omega)$ where $C^{0,\delta}$ denotes Hölder continuity. Suppose u has a zero of first order at x_0 so that $u = P_1(x-x_0) + \Phi$ in a neighbourhood of x_0 according to Theorem 1.1. (1.3) and (1.4) implies that for $\delta' < \delta \leq 1$

$$\lim_{x \to x_0} \frac{|u(x) - P_1(x-x_0)|}{|x-x_0|^{1+\delta'}} = 0$$

so that u is at x_0 'smoother' than at points for which $u \neq 0$. So the question arises whether the zero sets of solutions of Schrödinger equations are in fact smoother than the corresponding solutions.

Let us illustrate this with an explicit example. According to the theorem of Cauchy and Kowalewski there is a small disk

$$B_\rho = \{(x,y) \in \mathbb{R}^2 : x^2 + y^2 < \rho^2\}$$

such that

$$\Delta v = v \text{ in } B_\rho$$

with

$$v = x - y + \frac{1}{6}x^3 - \frac{1}{2}x^2 y + \text{ higher order terms}$$

and with $v(0,y) = -y$, $\frac{\partial v}{\partial x}(0,y) = 1$. Now let in B_ρ, u be defined by

$$u = \begin{cases} x - y & \text{for } x \leq 0 \\ v & \text{for } x > 0 \end{cases}$$

then $\Delta u = Vu$ with

$$V = V(x,y) = \begin{cases} 1 & x > 0 \\ 0 & x \leq 0 \end{cases}$$

and a simple calculation shows that the nodal line of u is given by

$$y = x \qquad \text{for } x \leq 0$$

$$y = x - \frac{1}{3}x^3 + O(x^5) \qquad \text{for } x > 0.$$

Hence $y(x)$ has a second derivative and one sided third derivatives. But u itself already has a jump in the second derivative for every (x,y) with $y = 0$ and $|x| \neq 0$.

Results on this additional regularity of nodal sets together with some proofs will be presented in this announcement, the full paper will appear elsewhere.

2. Regularity of nodal sets

Without loss of generality we consider (1.1) in $B_{R_0} = \{x \in \mathbb{R}^n : |x| < R_0\}$ and we assume $V \in K^{n,\delta}(B_{R_0})$. Let

(2.1) $$N_u = \{x \in B_{R_0} : u = 0\}$$

and let $N_u^{(1)} = \{x \in N_u : u \text{ vanishes of first order at } x\}$ so that for each $x_0 \in N_u^{(1)}$ there is a $P_1^{(x_0)}(x - x_0) \neq 0$ with

$$u(x) = P_1^{(x_0)}(x - x_0) + \Phi(x) \tag{2.2}$$

for $x \to x_0$ according to Theorem 1.1.

Theorem 2.1. *Pick $x_0 \in N_u^{(1)}$ and assume $\delta \leq 1$. Then for each $\delta' < \delta$ and for sufficiently small $\varepsilon > 0$, $N_u^{(1)} \cap B_\varepsilon(x_0)$ is a $C^{1,\delta'}$-hypersurface.*

Remarks.

(i) By a $C^{1,\delta'}$ hypersurface we mean that $N_u^{(1)} \cap B_\varepsilon(x_0)$ can be represented as the graph of a $C^{1,\delta'}(\mathbb{R}^{n-1})$ function.

(ii) Theorem 2.1 is sharp in the sense that $\delta' > \delta$ is not possible. We do not know whether $\delta' = \delta$ might be allowed.

(iii) We shall later discuss the case of smoother potentials, say $V \in K^{n,\delta}(\Omega)$ for $\delta \in (1, 2)$ or $V \in C^{k,\alpha}(\Omega)$. $C^{k,\alpha}$ denotes the usual Hölder spaces.

Sketch of the proof.

We first state a Lemma which is a sharpening of Theorem 1.1.

Lemma 2.1. *Let $x_0 \in N_u \cap B_{R_1}(\mathbf{0})$ with $R_1 = R_0/2$ and suppose $\sup_{x \in B_{R_0}} |u| = C_1$ then for every $\delta' < \delta$, there is a C_2 such that for $|x| < R_0$*

$$|u(x) - P_1^{(x_0)}(x - x_0)| \leq C_2 |x - x_0|^{1+\delta'}, \quad \textit{where} \\ C_2 = C_2(V, C_1, \delta - \delta', n, R_0) \tag{2.3}$$

Remark. The V-dependence can be made explicit via a suitable norm of V. The important fact is that C_2 does not depend on x_0. If x_0 happens to be a higher order zero of u then $P_1^{(x_0)}(x - x_0) \equiv 0$. The proof of Lemma 2.1 relies heavily on the techniques which have been developed in [HO2] in order to prove Theorem 1.1. Some additional technical complications arise, causing however no entirely new problems. Naturally a complete proof is, as already the proof of Theorem 1.1 somewhat involved.

Now define for $x_0, x_1 \in N_u$

$$(\nabla u)(x_i) = (\nabla P^{(x_i)})(x_i) = a_i, \quad i = 0, 1 \tag{2.4}$$

then it can be shown via Lemma 2.1

Lemma 2.2. *Let $x_0, x_1 \in N_u \cap B_{R_2}$, $R_2 = R_0/4$ then for $\delta' < \delta$ there is a constant C_3 such that*

$$|a_1 - a_2| \leq C_3 |x_0 - x_1|^{\delta'}. \tag{2.5}$$

with $C_3 = C_3(C_2)$, C_2 the constant given according to (2.3).

For later purposes we prove the following more general statement.

Lemma 2.2'. *Suppose $P_M^{(0)}$ and $P_M^{(1)}$ are polynominals of degree M and that*

$$|P_M^{(0)}(x) - P_M^{(1)}(x - x_1)| \leq c|x_1|^{M+\delta'}$$

for $|x| \leq 2|x_1|$. Then for every M-th partial derivative there exists a constant $C(M,n)$ such that

$$|\partial_M(P_M^{(0)}(x) - P_M^{(1)}(x - x_1))| \leq cC(M,n)|x_1|^{\delta'}$$

Proof. Let $Q_M(x) = P_M^{(0)}(x) - P_M^{(1)}(x - x_1)$. In the one-dimensional case $|Q_M(x)| \leq C|x_1|^{M+\delta'}$ implies via a classical inequality of Chebyshev that

$$|\frac{d^M}{dx^M}Q_M(x)| \leq C_M|x_1|^{\delta'}$$

To obtain the corresponding estimate for the n-dimensional case we consider directional derivatives of M-th order. There the one-dimensional estimate obviously holds. The partial derivatives can then be estimated by linear combinations of the directional derivatives [Bo].

We shall now proceed in the following way: we assume that $x_0 \in N_u^{(1)}$ and that

$$(\nabla u)(x_0) = (\lambda, 0, \ldots, 0) \equiv \lambda e_1, \quad \lambda \neq 0. \tag{2.6}$$

We shall first show that in a neighbourhood of x_0 the nodal set $u(x) = 0$ can be represented as the graph of a uniquely determined continuous function

$$\varphi : B_\gamma(\pi x_0) \subset \mathbb{R}^{n-1} \to \mathbb{R}$$

such that

$$u(\varphi(y), y) = 0 \quad \forall y \in B_\gamma(\pi x_0). \tag{2.7}$$

thereby π denotes the orthogonal projection from $\mathbb{R}^n$ to $S := \{x \in \mathbb{R}^n | x_1 = 0\}$ and $B_\gamma(\pi x_0) = \{y \in S || \pi x_0 - y| < \gamma\}$ with $\gamma > 0$ small enough.

Proposition 2.1. *For sufficiently small $\rho > 0$*

$$\pi : N_u \cap B_\rho(x_0) \to S$$

is injective.

Proof. We start with some rather obvious observations and definitions. Since $u(x_0) = 0$, $x_0 \in \partial G$ where $G = \{x \in B_{R_2} : u(x) > 0\}$. Let $\tilde{x} \in \partial G$. We say $\varepsilon_{\tilde{x}}$ is an $n-1$ dimensional affine hyperplane to ∂G at $\tilde{x}$ if for every sequence of points $x_i \in \partial G$ with $x_i \to \tilde{x}$

$$\text{dist}(x_i, \varepsilon_{\tilde{x}}) = o(|x_i - \tilde{x}|) \text{ for } i \to \infty.$$

Let $y \in \partial G$ and $d_y(x) := (x-y, (\nabla u)(y))$ then $\varepsilon_{x_0} = \{x \in \mathbb{R}^n : d_{x_0}(x) = 0\}$. Now define for $x \in \partial G \cap N_u^{(1)}$

$$(\tilde{\nabla} u)(x) = \frac{(\nabla u)(x)}{|(\nabla u)(x)|}$$

then by Lemma 2.2 it is straight forward to show that for small ρ'

$$((\tilde{\nabla} u)(x_0), (\tilde{\nabla} u)(x)) > \frac{1}{2} \tag{2.8}$$

for $x \in N_u \cap \overline{B}_{\rho'}(x_0)$ with $\overline{B}_{\rho'}(x_0) = \{x \in \mathbb{R}^n : |x - x_0| \leq \rho'\}$. Set $\rho = \rho'$ in Proposition 2.1.

Now suppose that Proposition 2.1 is wrong. Then there exist $\bar{x}, \underline{x} \in B_{\rho'}(x_0) \cap N_u, \bar{x} \neq \underline{x}$ such that $\pi(\bar{x}) = \pi(\underline{x}) := \tilde{x} = (0, \tilde{x}_2, \tilde{x}_3, \ldots, \tilde{x}_n)$. Let $E = \pi^{-1}(\tilde{x}) \cap \overline{B}_\rho(x_0) \cap N_u$. E is a closed set with cardinality ≥ 2. If E has an accumulation point y then $\pi^{-1}(\tilde{x}) \subset \varepsilon_y$, but $\varepsilon_y = \{x \in \mathbb{R}^n : (x - y, (\nabla u)(y)) = 0\}$ and this implies $((\tilde{\nabla} u)(x_0), (\tilde{\nabla} u)(y)) = 0$ contradicting (2.8). So there are $z_1, z_2 \in E$ where z_1, z_2 only differ in the first coordinate such that

$$g(z_1, z_2) = \{x \in \mathbb{R}^n : x = tz_1 + (1-t)z_2, t \in (0,1)\}$$

satisfies $g(z_1, z_2) \cap N_u = \emptyset$ implying $u(x) \neq 0 \quad \forall x \in g(z_1, z_2)$. But

$$((\nabla u)(x_0), (\nabla u)(z_j)) = \frac{\partial u}{\partial x_1}(x_0) \frac{\partial u}{\partial x_1}(z_j)$$

and

$$\operatorname{sgn} \frac{\partial u}{\partial x_1}(z_1) \neq \operatorname{sgn} \frac{\partial u}{\partial x_1}(z_2), \quad j = 1, 2,$$

hence $\operatorname{sgn} ((\tilde{\nabla} u)(x_0), (\tilde{\nabla} u)(z_1)) \neq \operatorname{sgn} ((\tilde{\nabla} u)(x_0), (\tilde{\nabla} u)(z_2))$ again contradicting (2.8). This proves the proposition.

Now we have to show the $\forall y \in B_\gamma(\pi x_0)$, γ small enough, there is a $t \in \mathbb{R}$ such that $(t, y) \in B_\rho(x_0) \cap N_u$. But this is an immediate consequence of the continuity of u : Denote $x_0 = (x_{01}, \ldots, x_{0n})$, let $y \in B_\gamma$ and $x_\pm := (x_{0,1} \pm \varepsilon, y)$ such that $x_\pm \in B_\rho(x_0)$. Since $\nabla u(x_0) = \lambda e_1$ and $u(x_0) = 0$, $\operatorname{sgn} u(x_{0,1} + \varepsilon, x_{0,2} \ldots x_{0,n}) \neq \operatorname{sgn} u(x_{0,1} - \varepsilon, x_{0,2} \ldots x_{0n})$ for ε small enough. Since u is continuous we also have $\forall y \in B_\gamma$, for γ sufficiently small, $\operatorname{sgn} u(x_{0,1} + \varepsilon, y) \neq \operatorname{sgn} u(x_{0,1} - \varepsilon, y)$. Hence by the intermediate value theorem there is a t with $|t - x_{0,1}| < \varepsilon$ such that $u(t, y) = 0$. This implies (2.7).

Further via an implicit function theorem [H, Satz 170.1] (which is not standard but ideal for our purposes) we conclude that $\varphi \in C^{1,\delta'}(B_\gamma)$ so that $N_u^{(1)}$ is indeed locally the graph of a $C^{1,\delta'}$ function.

We give now a brief discussion of the higher regularity of nodal sets if V is assumed to be more regular.

Theorem 2.2. *(i) Suppose (1.1) holds with $V \in K^{n,\delta}(\Omega)$ with $\delta \in$ (1,2]. Then $N_u^{(1)}$ is locally a $C^{2,\delta'}$-hypersurface for $\delta' < \delta - 1$.*

(ii) Suppose (1.1) holds with $V \in C^{k,\alpha}(\Omega)$ with $\alpha \in (0,1)$ then $N_u^{(1)}$ is locally a $C^{k+3,\alpha}$-hypersurface.

The idea of the proof is basically the same as for the proof of Theorem 2.1. However we have to replace Theorem 1.1 by a more detailed result.

Theorem 2.3.. *(i) Suppose (1.1) holds and* $V \in K^{n,\delta}(\Omega), \delta \in (1,2]$. *Let* $x_0 \in \Omega$ *then either there exist two harmonic homogenous polynomials* $P_M \neq 0, P_{M+1}$ *of degree* $M, M+1$ *respectively such that*

$$u(x) = P_M(x - x_0) + P_{M+1}(x - x_0) + \Phi(x)$$

with

$$\Phi(x) = O(|x - x_0|^{M+\delta'}) \quad \forall \delta' < \delta \text{ for } x \to x_0$$

or u *vanishes at* x_0 *faster than polynomially.*

(ii) Suppose (1.1) holds and

$$V \in C^{k,\alpha}(\Omega), \quad \alpha \in (0,1).$$

Let $x_0 \in \Omega$, *then there is a polynomial of degree* $M + k + 2$ *such that* $p(x) = P_M(x) + P_{M+1}(x) + p_1$ *with* P_M, P_{M+1} *again harmonic and homogenous of degree* $M, M+1$ *respectively and* $P_M \neq 0$, *and* $p_1(x)$ *vanishes at least of order* $M+2$ *at zero. We have then*

$$u(x) = p(x - x_0) + \Phi(x - x_0)$$

with

$$\Phi(x) = O(|x|)^{M+k+2+\alpha}$$

Remarks. (a) Under the conditions of part (ii) of this theorem strong unique continuation is well known. Also (ii) is related to the classical Schauder estimates, see e.g. [GT].

(b) The proof of Theorem 2.3 again uses the techniques of [HO2] but some iterations are necessary.

(c) For the coulombic case a more detailed version of Theorem 1.1 was recently shown in [HO2 S1] and [HO2 S2]. An investigation of the regularity of the nodal sets for this important case should be possible along the present lines.

Starting from Theorem 2.3 the proof of Theorem 2.2 follows the same ideas as the proof of Theorem 2.1. So one first proves a suitable analog of Lemma 2.1, uses Lemma 2.2' and proceeds essentially as we did above in order to prove Theorem 2.1.

References

[AS] M. Aizenman, B. Simon,, *Brownian motion and Harnack inequality for Schrödinger operators*, Commun Pure Applied Mathematics **35** (1982), 209-273.

[BO] J. Boman, *Differentiability of a function and of its composition with functions of one variable*, Math. Scand. **20** (1967), 249-286.

[GT] D.Gilbarg, N.S.Trudinger, *Elliptic partial differential equations*, Springer, Berlin, 1983.

[HO2] M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, *Local properties of solutions of Schrödinger equations*, Comm. PDE **17** (1992), 491-522.

[HO2S1] M.Hoffmann-Ostenhof, T.Hoffmann-Ostenhof and H.Stremnitzer, *Electronic wavefunctions near coalescence points*, Phys. Rev. Letters **68** (1992), 3857-3860.

[HO2S2] M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof and H. Stremnitzer, *Local properties of Coulombic wavefunctions*, submitted for publication.

[H] H. Heuser, *Lehrbuch der Analysis Teil 2*, B. G. Teubner, Stuttgart, 1988.
[S] B. Simon, *Scrödinger semigroups*, Bull. Am. Math. Soc. **7** (1982), 447-526.

M. HOFFMANN-OSTENHOF: INSTITUT FÜR MATHEMATIK, UNIVERSITÄT WIEN, STRUDLHOFGASSE 4, A-1090 WIEN, AUSTRIA

T. HOFFMANN-OSTENHOF: INSTITUT FÜR THEORETISCHE CHEMIE, UNIVERSITÄT WIEN, WÄHRINGER STRASSE 17, A-1090 WIEN, AUSTRIA AND INTERNATIONAL ERWIN SCHRÖDINGER INSTITUTE FOR MATHEMATICAL PHYSICS, PASTEURGASSE 6/7, A-1090 WIEN, AUSTRIA
E-mail address: hoho@itc.univie.ac.at

N. NADIRASHVILI: INTERNATIONAL ERWIN SCHRÖDINGER INSTITUTE FOR MATHEMATICAL PHYSICS, PASTEURGASSE 6/7, A-1090 WIEN, AUSTRIA AND INSTITUTE OF EARTH PHYSICS, MOSCOW, RUSSIA