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ASYMPTOTIC PROPERTIES OF NODES OF SOLUTIONS TO SCHRÖDINGER EQUATIONS

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In this talk we shall be concerned with real valued solutions ψ of Schrödinger equations $(-\Delta + V - E)\psi = 0$ in a domain $\Omega \subset \mathbb{R}^n$, $n \geq 2$, under suitable assumptions on V and E. In the literature there are not many results about nodal properties of such solutions. We mention only the classical global result of Courant [6], and the local results of Bers [2], Cheng [5] and Caffarelli and Friedmann [3].

For Ω unbounded the nodal set of ψ, i.e. $\{x \in \Omega | \psi(x) = 0\}$ is in general unbounded and it is natural and interesting to investigate the asymptotic properties of ψ in relation with its nodes. Such investigations were performed by the present authors (partly in collaboration with J. Swetina) in a series of papers (for $n = 2$ in [10,12], and for $n \geq 3$ in [11,13]). We first give a survey of some of the results obtained there. Then we announce a new local result about the geometry of the nodal set of such solutions ψ. For its proof methods developed in [13] and results of Bers [2] are used.

First we consider real valued $W^{2,2}$-solutions $\psi(x)$ of

$$(-\Delta + V - E)\psi = 0 \text{ for } x \in \Omega_R, \qquad \Omega_R = \{x \in \mathbb{R}^n | |x| = r > R\}, R > 0, n \geq 2. \quad (1)$$

Here the Sobolev space $W^{2,2}(\Omega_R)$ is defined as in [8]. We assume that

$$E < 0 \quad (2)$$

and that $V(x)$ satisfies the following conditions:

$$V \text{ is real valued and continuous in } \bar{\Omega}_R, \quad (A.1)$$

$$\lim_{|x| \to \infty} V(x) = 0. \quad (A.2)$$

(2), (A.1) and (A.2) imply that we can choose R so that

$$\inf_{x\in\Omega_R}(V(x)-E)>0. \tag{A.3}$$

The above assumptions on V imply that $C_0^\infty(\Omega_R)$ is a form core for the quadratic form associated to $-\Delta+V-E$ and its Friedrichs extension is a positive definite selfadjoint operator. This guarantees that given $\psi=\varphi$ on $\partial\Omega_R$ with φ continuous in a neighbourhood of $\partial\Omega_R$, the corresponding Dirichlet problem (1) is uniquely solvable [8].

Before we specify our assumptions on V further, we should mention that there is a rich literature on the asymptotics of solutions of Schrödinger equations. See for instance [1,7,13] and references therein.

We split V so that

$$V(x)=V_1(r)+V_2(x) \tag{A.4}$$

and assume that V_1 and V_2 satisfy the conditions (A.1 – A.3) separately. Furthermore we assume that in Ω_R

$$\left.\begin{array}{ll}V_1 \text{ is continuously differentiable and} & \\ |\frac{dV_1}{dr}|\leq cr^{-1-\epsilon} & \text{for some } c,\epsilon>0\end{array}\right\} \tag{A.5}$$

and that

$$|V_2|\leq c_0r^{-1-\gamma} \qquad \text{for some } c_0,\gamma>0. \tag{A.6}$$

Next we consider a radial comparison problem to (1),

$$\left.\begin{array}{ll}(-\Delta+V_1-E)v=0 & \text{in } \Omega_R \\ \text{with } v\in L^2(\Omega_R),\ v=v(r) \text{ and } v>0 \text{ in } \Omega_R. & \end{array}\right\} \tag{3}$$

We write $\psi=\psi(ry)$ where $y=\frac{x}{r}\in S^{n-1}$ (S^{n-1} the unit sphere in $\mathbf{R}^n$) and define

$$\psi_{av}(r)=\left(\int_{S^{n-1}}\psi^2d\sigma\right)^{1/2}$$

(where $d\sigma$ denotes normalized integration over S^{n-1}) and

$$u=\psi/v,$$

then we have (see [9,11])

Theorem 1: Let $\psi\not\equiv 0$ be given according to (1), $E<0$, and let $V=V_1(r)+V_2(x)$ satisfy the foregoing conditions (A). Then for some $c_-,c_+>0$

$$|\psi|\leq c_+v, \qquad c_-v\leq\psi_{av} \qquad \text{for } r\geq R$$

and

$$A(y)\equiv\lim_{r\to\infty}u(ry) \text{ exists and } A \text{ is continuous.}$$

Theorem 1 permits us to investigate various asymptotic properties of u, from which corresponding results follow for the intrinsically defined function ψ/ψ_{av}.

To illustrate that the asymptotic behaviour of u (resp. ψ/ψ_{av}) is already a nontrivial problem for a spherical symmetric potential (i.e. $V_2 \equiv 0$) we use an example of quantum mechanics, the Schrödinger equation for the Hydrogen atom

$$(-\Delta - \frac{2}{r} - E_n)\psi_n = 0, \qquad E_n = -\frac{1}{n^2},$$

with $\psi_n \in L^2(\mathbf{R}^3)$, $n = 1, 2, \ldots$, an eigenfunction corresponding to the n^2-fold degenerated eigenvalue E_n. It is well-known that ψ_n can be written as

$$\psi_n = \sum_{\ell=0}^{n-1} \sum_{m=-\ell}^{\ell} c_{\ell,m}^{(n)} f_\ell^{(n)}(r) Y_\ell^{(m)}(y),$$

where the $Y_\ell^{(m)}$ are the usual surface harmonics. The $f_\ell^{(n)}$ satisfy on $(0,\infty)$ the ordinary differential equation

$$(-\frac{d^2}{dr^2} - \frac{2}{r} + \frac{\ell(\ell+1)}{r^2} - E_n) r f_\ell^{(n)} = 0,$$

and show the ℓ-independent asymptotics

$$f_\ell^{(n)}(r) \sim r^{1/\sqrt{|E_n|}-1} e^{-\sqrt{|E_n|}r} \qquad \text{for } r \to \infty.$$

Then with $u_n = \psi_n / f_0^{(n)}$ and $A_n(y) = \lim_{r\to\infty} u_n$, $n \in \mathbf{N}$, we obtain explicit examples for which the behaviour of the nodal surfaces is nontrivial for $r \to \infty$.

For the following we need additional assumptions on the decay and regularity of V_2. We require that for $\bar{R} > R$ and

$$\left.\begin{array}{l} \text{for some } \alpha > \frac{1}{2},\ r^{1+\alpha} V_2(ry) \in C_u^\omega(S^{n-1}), \\ \text{i.e. } \{r^{1+\alpha} V_2(r\cdot), r \geq \bar{R}\} \text{ is a uniformly bounded set} \\ \text{of } C^\omega(S^{n-1}) \text{ functions } (C^\omega \text{ means real analytic).} \end{array}\right\} \qquad (B)$$

We first state our results for dimension <u>$n = 2$</u>:

It will be convenient to use polar coordinates $x_1 = r\cos\omega$, $x_2 = r\sin\omega$, $\omega \in [-\pi, \pi]$. Further we write $\psi = \psi(r,\omega)$ and $A = A(\omega)$.

Theorem 2: Suppose the assumptions of Theorem 1 hold and V_2 satisfies condition (B), then

(i) $u(ry) \in C_u^\omega(S^1)$, $A \in C^\omega(S^1)$ and $A \not\equiv 0$. Further for $k \in \mathbf{N} \cup \{0\}$

$$\left|\frac{\partial^k}{\partial\omega^k}(u(r,\omega) - A(\omega))\right| \leq c_k r^{-a}, \qquad a = \min(1, \alpha), \qquad (4)$$

in $\Omega_{\bar{R}}$ for $\bar{R} > R$ large enough with some $c_k < \infty$ (not depending on r).

(ii) Let $\beta \in (0, 1/2)$ and $\mathcal{D}_\beta = \{x \in \Omega_{R_\beta} \| \omega| < r^{-\beta}\}$, R_β sufficiently large. Suppose $A(0) = 0$, so that for some $M \in \mathbf{N}$ and for $|\omega|$ small, $A(\omega) = \omega^M + O(\omega^{M+1})$. Then for some $\delta, \nu > 0$ we have in $\mathcal{D}_\beta$

$$u(r, \omega) = (2b)^{-M} r^{-M/2} H_M(b\sqrt{r}\omega)(1 + O(r^{-\nu})) + O(r^{-M/2-\delta}), \qquad (5)$$

where $b = (|E|/4)^{1/2}$ and H_M denotes the Hermite polynomial of degree M.

Corollary 1: Choosing $\omega = z/(b\sqrt{r})$ and denoting

$$U_M(r, z) = r^{M/2} u(r, \frac{z}{b\sqrt{r}})$$

(5) implies

$$U_M(r, z) \to (2b)^{-M} H_M(z) \text{ for } r \to \infty, \forall z \in \mathbf{R}. \qquad (6)$$

The proof of Theorem 2 is given in [10]. We note that the proof of part (ii) is based on iterations of an integrodifferential equation for u.

Investigating the properties of $U_M(r, z)$ further it was shown in [12] that for large r the nodal set of ψ consists of non intersecting nodal lines which look asymptotically either like straight lines or like branches of parabolas. Specifically we have

Theorem 3: Suppose the assumptions of Theorem 2 hold. Assume $A(0) = 0$ with

$$A(\omega) = \omega^M + d\omega^{M+1} + O(\omega^{M+2}) \qquad \text{for } |\omega| \text{ small}$$

for some $d \in \mathbf{R}$ and $M \in \mathbf{N}$. Let $z_i \in \mathbf{R}$ for $1 \le i \le M$ denote the zeros of the Hermite polynomial H_M, i.e. $H_M(z_i) = 0$ for $1 \le i \le M$.

Then for $\epsilon > 0$ sufficiently small and R_ϵ large the nodal set of ψ in $D_\epsilon \equiv \{x \in \Omega_R | r > R_\epsilon, |\omega| < \epsilon\}$ consists of M nodal lines (corresponding to the M zeros of H_M). They admit a representation in cartesian coordinates ($(x_1, x_2) \in \mathbf{R}^2$) denoted by $x_2 = G_i(x_1)$ for $1 \le i \le M$. Therefore denoting $\psi = \psi(x_1, x_2)$, $\psi(x_1, G_i(x_1)) = 0$ for $1 \le i \le M$. For all i, G_i is continuously differentiable and the nodal lines have the following asymptotic behaviour:

For $M \ge 2$ and $z_i \ne 0$

$$G_i(x_1) = (\frac{z_i}{b} + o(1))\sqrt{x_1} \qquad \text{for large } x_1$$

with $b = (|E|/4)^{1/4}$. Further if $z_i > 0$ (< 0), then G_i is strictly monotonically increasing (decreasing) for large x_1.

For M odd, $H_M(0) = 0$ and without loss let $z_1 = 0$, then

$$G_1(x_1) = \frac{d}{\sqrt{|E|}} + o(1) \qquad \text{for large } x_1.$$

For dimensions $n \ge 3$ the structure of the nodal set near infinity of a solution ψ can show much more complicated patterns than for $n = 2$, due to the fact that the nodal set of A will be usually an $(n-2)$-dimensional object. Though there is an asymptotic expansion for u analogously to Theorem 2 (given in [11]), where linear combinations of products of Hermite polynomials occur, it seems to be no longer possible in general to characterize the nodal surfaces as in Theorem 3 the nodal lines. But in [13] we obtain results on the asymptotics of ψ/ψ_{av} in relation with the asymptotic behaviour of the nodal domains of ψ:

Let $r_0 \geq R$ and let $\mathcal{N}_{r_0} = \{x \in \Omega_{r_0} | \psi(x) = 0\}$. A component D_{r_0} of $\Omega_{r_0} \setminus \mathcal{N}_{r_0}$ will be called a nodal domain of ψ in Ω_{r_0}. Further we define for $r \geq R$

$$S(r) = \{y \in S^{n-1} | ry \in D_{r_0}\}$$

and denote $|S(r)| = \int_{S(r)} d\sigma$.

The main results for $n \geq 3$ are:

Theorem 4: Let E, V and ψ be given as in Theorem 1 and let V_2 satisfy condition (B). Let D_{r_0} be an unbounded nodal domain of ψ, then for some $\gamma geq 0$ and $c > 0$

$$\psi_0/\psi_{av} \geq cr^{-\gamma} \qquad \forall r \geq r_0, \qquad \text{where } \psi_0 = (\textstyle\int_{S(r)} \psi^2 d\sigma)^{1/2}. \tag{7}$$

Theorem 5: Let $B_r = \{x \in \mathbb{R}^n | |x| < r\}$, then under the same assumptions as in Theorem 4

$$\underline{\lim}_{r\to\infty} \frac{\ln(\mathrm{Vol}(D_{r_0} \cap B_r))}{\ln r} \geq \frac{n+1}{2}. \tag{8}$$

We note that for $n = 2$ the result analogous to (8) is

$$\lim_{r\to\infty} \frac{\ln(\mathrm{Vol}(D_{r_0} \cap B_r))}{\ln r} \in \{\frac{3}{2}, 2\}$$

as a consequence of Theorem 3.

The main ideas of the proofs of Theorem 4 and 5 (given in [13]) are the following:

By application of the n-dimensional analogue to Theorem 2(i) (derived in [11]) it can be seen that $\underline{\lim}_{r\to\infty} |S(r)| > 0$ or $\lim_{r\to\infty} |S(r)| = 0$. Since in the first case Theorem 4 is trivial, let $|S(r)| \to 0$ for $r \to \infty$. We define

$$\lambda^2(r) = \inf_{\varphi \in C_0^\infty(S(r))} \frac{\int |L\varphi|^2 d\sigma}{\int |\varphi|^2 d\sigma}$$

where $-L^2$ is the Laplace-Beltrami operator on S^{n-1}. Then $\lambda^2(r) \to \infty$ for $r \to \infty$ (e.g. by the Faber-Krahn inequality [4]).

It is not difficult to show that $\tilde{\psi}_0 = r^{(n-1)/2}\psi_0$ satisfies in the distributional sense

$$\left(-\frac{d^2}{dr^2} + V_1 - E + \inf_{y \in S^{n-1}} V_2(ry) + \frac{(n-1)(n-3)}{4r^2} + \frac{\lambda^2(r)}{r^2}\right)\tilde{\psi}_0 \leq 0 \tag{9}$$

for $r > R$, whereas the proof of

Lemma 1: There exists a $\gamma \geq 1$ such that

$$\underline{\lim}_{r\to\infty}\lambda^{2\gamma}(r)(\frac{\psi_0}{v})(r) > 0 \tag{10}$$

is rather involved. We mention that thereby the analyticity of A and n-dimensional estimates analogous to (4) are heavily used. Specifically it is shown that $2\gamma = M + (n-1)/2$, where M is the highest order of the zeros of A.

From (9) and (10) it follows via linear and nonlinear comparison techniques for differential inequalities that

$$\underline{\lim}_{r\to\infty}\lambda^2(r)r^{-1} < \infty \tag{11}$$

which finally again by application of Lemma 1 leads to (7).

For the proof of Theorem 5 we observe that the "growth" of the nodal domain considered is connected with the asymptotics of $\lambda^2(r)$ by

$$\mathrm{Vol}(D_{r_0} \cap B_r) \geq c_1 \int_{r_0}^{r} |S(x)|x^{n-1}dx \geq c_2 \int_{r_0}^{r} (\frac{x}{\lambda(x)})^{n-1}dx.$$

Roughly speaking: $\lambda^2(r)$ cannot increase "too much", since this would imply via inequality (9) that ψ decays "too much" contradicting Theorem 5.

Finally we announce a result on the behaviour of a local solution of a Schrödinger equation in a neighbourhood of a zero [14]. The result is derived by a suitable modification of the methods developed to prove Theorem 4, and by making use of a theorem of Bers [2].

$$\left.\begin{array}{l}\text{Let } \Omega \subset \mathbf{R}^n,\ (n \geq 2) \text{ be a domain with } x_0 \in \Omega.\\ \text{Let } V \in C^\infty(\Omega) \text{ and } \psi \not\equiv 0,\ \psi \in C^\infty(\Omega) \text{ satisfying}\\ (-\Delta + V)\psi = 0 \text{ in } \Omega \text{ and } \psi(x_0) = 0.\\ \text{Without loss we assume } x_0 = \mathcal{O}.\end{array}\right\} \tag{12}$$

Under the above asssumptions Bers' result tells us that there exists a homogenous harmonic polynomial $P_M(x) \not\equiv 0$, of degree $M \geq 1$ such that for $0 < \epsilon < 1$

$$\frac{\partial^\ell(\psi - P_M)(x)}{\partial x_1^{i_1}\ldots\partial x_n^{i_n}} = O(|x|^{M-\ell+\epsilon}) \tag{13}$$

for $\ell = 0, 1, 2, \ldots, M$, where $\sum_{j=1}^{n} i_j = \ell$.

For the 2-dimensional case it is known (see e.g. [5]) that the nodal lines of ψ, which pass through the origin, form an equiangular system as the straight nodal lines of P_M do.

For dimensions $n \geq 3$ the situation is more complicated: Since we can write $P_M(x) = r^M Y_M(y)$, (Y_M a surface harmonic) it follows from the above that

$$\lim_{r\to 0} r^{-M}\psi(ry) = Y_M(y) \qquad \forall y \in S^{n-1}. \tag{14}$$

But it is a priori not clear how the nodal set of ψ in a neighbourhood of the origin is determined by the nodal set of Y_M. So the question arises whether there exists a nodal domain D_{r_0} of ψ, for which the corresponding $S(r)$ "shrinks" as $r \to 0$ into a subset of the nodal set of Y_M (due to the zeros of Y_M of order ≥ 2). As before D_{r_0} denotes a component of $B_{r_0} \setminus \{x \in \Omega | \psi(x) = 0\}$, where $B_{r_0} = \{x \in \mathbf{R}^n | |x| < r_0\}$ with r_0 sufficiently small, and again $S(r) = \{y \in S^{n-1} | ry \in D_{r_0}\}$. The question above is answered by

Theorem 6 [14]: Let ψ be given according to (12) and satisfy (14). Let D_{r_0} denote a nodal domain of ψ with $\mathcal{O} \in \partial D_{r_0}$ and denote $\psi_0 = (\int_{S(r)} \psi^2 d\sigma)^{1/2}$, then $\psi_0 r^{-M}$ and $|S(r)|$ have for $r \to 0$ non zero finite limits.

Corollary: This implies that the number of nodal domains of ψ, whose boundaries hit the origin, is smaller than or equal to the number of the nodal domains of Y_M.

The case $r \to 0$ in Theorem 6 parallels in some sense the case $r \to \infty$ in Theorems 4 and 5, and it turns out that Theorem 6 can be proven by following the ideas of the proof of Theorem 4 with suitable modifications.

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