BEHAVIOUR OF THE WAVE FUNCTION NEAR THE ORIGIN IN THE
RADIAL CASE

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ABSTRACT

We give one more proof in two and three space dimensions that the irregular solution of the
Schrödinger equation, for zero angular momentum, is in fact the solution of an equation con-
taining an extra “delta function”. We propose another criterium to eliminate the irregular
solution which is to require the validity of the virial theorem of which we give a general proof
in the classical and quantum cases.

1 Introduction

These pedagogical remarks were stimulated by an exchange of ideas with Yves Cantelaube.

We re-examine the following question: in the case of a central potential why choose the
“regular solution” at the origin of the Schrödinger equation, while the irregular solution may
also be square integrable? It is indeed easy to show that for any negative energy there exists,
under weak conditions on the potential, a solution exponentially decreasing at infinity which,
outside the conventional eigenvalues, is irregular at the origin and square integrable. This is
explicitly demonstrated in Section 2. I would just like first to present, in my own way, the
standard argument (Dirac[1], Van Hove[2], Cohen-Tannoudji et al.[3], Basdevant et al.[4]) that
the irregular solution is not a solution of the original Schrödinger equation but a solution of an
equation containing an extra delta function. Then, I would like to propose another criterium:
the violation of the virial theorem by the irregular solution. I refuse to enter into the questions of
self-adjointness. You prove that a certain operator is self-adjoint on a certain domain. Choosing
the domain is more or less choosing the answer.
2 Proof of the existence of singular, normalizable solutions

Consider the reduced Schrödinger equation in three dimensions for $\ell = 0$:

$$\left(-\frac{d^2}{dr^2} + V(r) - E\right)u = 0$$

$$u = r\psi.$$  \hspace{1cm} (1)

Assume $V \to 0$ for $r \to \infty$. Then for $E < 0$, there exists $R$ such that

$$V(r) - E \geq K^2 > 0 \text{ for } r \geq R.$$  \hspace{1cm} (2)

Consider the solution such that

$$u'(R) = 0.$$  

By comparing Eq. (1) with

$$\left(-\frac{d^2}{dr^2} + K^2\right)u = 0$$  \hspace{1cm} (3)

it is easy to see that

$$u(r) > u(R) \cosh K(r - R)$$

for $r > R$,  \hspace{1cm} (4)

and that $u(r)$ is increasing.

We can define another solution of Eq. (1), $v$ which has a constant Wronskian with $u$:

$$u'v - v'u = 1$$  \hspace{1cm} (5)

A particular solution of (5) is

$$v = u \int_r^\infty \frac{dr'}{u^2(r')}$$  \hspace{1cm} (6)

From (4) we get

$$v < \int_r^\infty \frac{dr'}{u(R)\cosh K(r - R)} = \frac{2}{K} \exp - \frac{K(r - R)}{u(R)}$$  \hspace{1cm} (7)

The solution $v$ can be continued for $r < R$ till the origin.

Equation (1) can be written in integral form as

$$v = v(R_0) + (r - R_0)v'(R_0) - \int_r^{R_0} (r' - r)(V(r') - E)v(r')dr'$$  \hspace{1cm} (8)

Hence, for $r < R_0$,

$$M(r, R_0) < |v(R_0)| + R_0|v'(R_0)|$$

$$+ \int_0^{R_0} r'[|V(r')| + |E|]M(r, R_0)dr'.$$
where
\[ M(r, R_0) = \sup_{r < r' < R_0} |v(r')|. \]

If
\[ \int_0^c r' |V(r')| dr' < \infty, \]
we can choose \( R_0 \) in such a way that
\[ \int_0^{R_0} r' |V(r')| + |E| dr' < \epsilon < 1 \]
and hence
\[ M(r, R_0) < \frac{|v(R_0)| + R_0 |v'(R_0)|}{1 - \epsilon} \]
so \( |v(r)| \) has a fixed bound, independent of \( r \).

Condition (9) is only sufficient. In particular one can have acceptable oscillating potentials as shown by Chadan and collaborators [5] which violate (9).

Now, since the wave function is given by
\[ \psi = \text{const. } r u, \]
it is clear that \( \psi \) is normalizable because \( \int |\psi|^2 d^3r \) converges both at the origin and at infinity. This is valid for any \( E < 0 \), in particular for a value \( E \) which is not a conventional eigenvalue (for which \( v \) would tend to zero at the origin).

## 3 The delta function in the radial case with three-dimensions

We want to prove that the solution of the Schrödinger equation
\[ \psi = \frac{1}{r} u \]
cannot behave like \( \frac{1}{r} \) at the origin.

Take
\[ f = \frac{1}{\sqrt{r^2 + a^2}} \]
\[ \Delta f = \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} f = -3 \frac{a^2}{(r^2 + a^2)^{5/2}} = -g \]
Let us prove that for \( a \to 0 \), \( g \) tends to \( 4\pi \delta^3/(\vec{r}) \).

1) for \( r = 0 \), \( g \to \infty \) for \( a \to 0 \)
2) for any $r > 0$, $g \to 0$, for $a \to 0$

3) $\int d^3r g(\vec{r}) = 4\pi \int_0^\infty \frac{3a^2r^2dr}{(a^2+r^2)^{5/2}} = 4\pi$.

Hence for

$$a \to 0, g \to 4\pi \delta^3(\vec{r})$$

$$\Delta_3(-\frac{1}{r}) = +4\pi \delta^3(\vec{r}).$$

(14)

Notice that the sign is obvious since $-1/r$ is a subharmonic function. Hence, as announced the irregular solution of the Schrödinger equation is not acceptable.

4 The case of two-dimensions

The regular solution for zero azimuthal angular momentum behaves like 1, the irregular solution behaves like $\ln r$. We use

$$f = \ln \sqrt{r^2 + a^2} = \frac{1}{2} \ln(r^2 + a^2)$$

(15)

$$\Delta f = \frac{11}{2r} \frac{dr}{dr} \frac{d}{dr} \ln(r^2 + a^2)$$

$$= \frac{2a^2}{(r^2 + a^2)^2} = g$$

(16)

Let us prove that $g$ is proportional to a delta function in the limit $a \to 0$

1) again $g \to \infty$ for $r = 0$ $a \to 0$

2) $g \to 0$ for $r > 0$ $a \to 0$

3) $\int d^2r g = 2\pi \int rdr \frac{2a^2}{(r^2 + a^2)^2} = 2\pi$

(17)

Hence

$$g \to 2\pi \delta^2(\vec{r})$$

(18)

for $a \to 0$. Again the sign is correct because $\ln r$ is subharmonic since $\ln r$ tends to MINUS infinity for $r \to 0$.  

4
5 The virial theorem

The virial theorem should hold classically and “quantically”. Let me remind the classical proof in the general case.

If \( \vec{F}_i = -\vec{\nabla}_i V(x_1, x_2, \ldots, x_n) \),

\begin{equation}
\text{n_i} \frac{d^2 \vec{x}_i}{dt^2} = -\vec{\nabla}_i V . \tag{19}
\end{equation}

Newton’s equations are

\begin{equation}
m_i \frac{d^2 \vec{x}_i}{dt^2} = -\vec{\nabla}_i V . \tag{20}
\end{equation}

Hence

\begin{equation}
\sum n_i \frac{d^2 \vec{x}_i}{dt^2} = -\sum \vec{x}_i \vec{\nabla}_i V \tag{21}
\end{equation}

and

\begin{equation}
-\int_0^T \sum n_i \vec{x}_i \cdot \frac{d^2 \vec{x}_i}{dt} = -\sum n_i \vec{x}_i \frac{d\vec{x}_i}{dt} \bigg|_0^T + \int_0^T \sum n_i \left( \frac{d\vec{x}_i}{dt} \right)^2 dt = \int_0^T \sum \vec{x}_i \vec{\nabla}_i V dt \tag{22}
\end{equation}

So if you deal with a confined system (big problem!)

\begin{equation}
\lim_{T \to \infty} \frac{1}{T} \left( \sum n_i \vec{x}_i \frac{d\vec{x}_i}{dt} \right)_0^T = 0 . \tag{23}
\end{equation}

Strictly speaking, we know only that the above parenthesis is bounded for almost every \( T \) if the \( x_i \)'s are bounded. This inconvenient could be avoided by smoothing the cut-off at \( T \) in the integrals.

With this caveat, the average over time of the kinetic energy is:

\begin{equation}
\lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{1}{2} \sum n_i \left( \frac{d\vec{x}_i}{dt} \right)^2 dt = \lim_{T \to \infty} \frac{1}{T} \int_0^\infty \frac{\sum \vec{x}_i \vec{\nabla}_i V}{2} dt . \tag{23}
\end{equation}

If some particles escape at infinity with velocities \( \vec{v}_i \) (nobody knows if this will happen in the solar system), we get

\begin{equation}
\lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{1}{2} \sum n_i \left( \frac{d\vec{x}_i}{dt} \right)^2 dt = \sum \frac{1}{2} m_i \vec{v}_i^2 + \lim_{T \to \infty} \frac{1}{T} \int_0^T \sum \vec{x}_i \vec{\nabla}_i V dt \tag{24}
\end{equation}

and hence we have an inequality instead of an equality.

In the quantum case, the average over time of the kinetic energy is replaced by an average over space of the kinetic energy operator. For the radial case the virial theorem can be proved by hand, but, following Thirring[6], the best general proof uses scaling. Consider the Hamiltonian

\begin{equation}
H = -\sum \frac{\Delta_i}{2m_i} + V(x_1, x_2, \ldots, x_n) , \quad H\psi_k = E_k\psi_k \tag{25}
\end{equation}

if we change the scale \( x_i \to \lambda x_i \), the energy will be unchanged for

\begin{equation}
H_\lambda = -\frac{1}{\lambda^2} \sum \frac{\Delta_i}{2m_i} + V(\lambda x_1, \ldots, \lambda x_N) \tag{26}
\end{equation}

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so if we consider the Hamiltonian

$$\lambda^2 H_\lambda = - \sum \frac{\Delta_i}{2m_i} + \lambda^2 V(\lambda x_1, ..., \lambda x_N),$$

(27)

the energy levels $\epsilon_k$ are

$$\epsilon_k(\lambda) = \lambda^2 E_k$$

(28)

so, for $\lambda = 1$, by the Feynman-Hellman theorem,

$$\frac{d\epsilon_k}{d\lambda} = 2E_k = 2\langle V(x_1, ..., x_N) \rangle + \langle \Sigma \vec{x}_i \vec{\nabla}_i V(x_1, ..., x_N) \rangle,$$

(29)

so

$$E_k = \langle V(x_1, ..., x_N) \rangle + \frac{1}{2} \langle \Sigma \vec{x}_i \vec{\nabla}_i V \rangle$$

and since $E_k = \langle T \rangle + \langle V \rangle$, $T$ being the kinetic energy operator,

$$\langle T \rangle = \frac{1}{2} \langle \Sigma \vec{x}_i \vec{\nabla}_i \rangle.$$  

(30)

**Remark:** the choice of the origin is irrelevant because $\langle \vec{a} \cdot \vec{\nabla} V \rangle = 0$ if $\vec{a}$ is a fixed vector. This can be verified in an elementary way, using the Schrödinger equation.

### 6 Virial theorem in the three-dimensional quantum case

First, we would like to give also the “pedestrian” proof of the virial theorem in the 3 dimensions radial case, to show the importance of the prescription $u = 0$.

Take the Schrödinger equation

$$-u'' + Vu = Eu,$$

(31)

multiply by $u$ and integrate. This gives

$$-uu'\bigg|_0^\infty + \int_0^\infty u'^2dr + \int V u^2dr = E \int u^2dr$$

(32)

multiply also by $2ru'$ and integrate. This gives

$$-ru'^2\bigg|_0^\infty + \int_0^\infty u'^2dr + rVu^2\bigg|_0^\infty - \int_0^\infty \left(V u^2 + r \frac{dV}{dr} u^2\right) dr$$

$$= Er u^2\bigg|_0^\infty - E \int u^2dr$$

(33)

Assume that $u$ and $u'$ vanish at $r \to \infty$. Adding up the 2 equations, we get

$$\lim_{r \to 0} \left( uu' + ru'^2 - rVu^2 \right) + 2 \int u'^2dr = \int_0^\infty r \frac{dV}{dr} u^2dr$$

(34)
If \( u(r) \sim r \) for \( r \to 0 \) and if \( u'(0) \) is finite, we get the virial theorem, if \( u(0) = 1 \) and if \( u'(0) \) is not zero, the virial theorem is violated. If \( \int_{0}^{r} V(r')dr' \to \pm \infty \) for \( r \to 0 \), it is impossible to have \( u'(0) = 0 \) because \( |u'(r)| \to \infty \) for \( r \to 0 \), and this dominates \( \lim rV \).

If \( V \) is integrable near the origin, one can save the virial theorem by taking \( u'(0) = 0 \). This, however, is equivalent to looking at a symmetric one dimensional potential \( V(x) = V(-x) \) and looking at the even levels. Notice that any other boundary condition at the origin violates the virial theorem.

Now the point is that if the virial theorem holds at the classical level, it should hold too at the quantum level, according to the sacro-sanct “correspondence principle” of Bohr.

In the case of Coulomb interactions, we see that
\[
\frac{1}{2}r \frac{d}{dr}V(r) = -\frac{1}{2} \frac{1}{r}
\]
so
\[
\langle T \rangle = -\frac{1}{2} \langle V \rangle = -E.
\]
Taking a solution irregular at the origin for the case of Coulomb in 3 dimensions gives
\[
\langle V \rangle \sim -\int r^2 dr \frac{1}{r} \times \frac{1}{r^2} = -\infty
\]
and the virial theorem is completely violated. The same is true for potentials more singular than Coulomb.

For the radial case, we have seen that we can save formally the virial theorem if \( V \) is integrable at the origin and \( u(0) = 1 \) only if \( u'(0) = 0 \). This corresponds to an unphysical self-adjoint extension. Indeed while \( \int u^2 dr \) is finite, \( \int |\nabla \psi|^2 d^2 r \) diverges.

## 7 Virial theorem in the two-dimensional quantum case

In the radial case, the possible behaviour of the wave function at the origin are
\[
\psi \sim c, \psi \sim \ln r \quad (35)
\]
If \( \psi \to c \), the kinetic energy is given by
\[
\langle T \rangle = \int |\nabla \psi|^2 dr^2 = -\int \psi \Delta \psi d^2r = \frac{1}{2} \int \left( r \frac{dV}{dr} \right) \psi^2 d^2r,
\]
and the virial theorem is satisfied. More specifically, using the reduced wave function
\[
u = \sqrt{2\pi r},
\]
(37)
which satisfies
\[-u'' - \frac{u}{4r^2} + Vu = Eu\] (38)
and using the same strategy as in the three-dimensional case, we get
\[
\langle T \rangle = \frac{1}{2} \lim_{r \to 0} \frac{|u(r)|^2}{r} + \int \left( u^2 - \frac{u^2}{4r^2} \right) r dr = \frac{1}{2} \int r \frac{dV}{dr} u^2 dr
\] (39)
If on the other hand, \( \psi \sim \ln r \) near the origin, \( \nabla \psi \sim \frac{1}{r} \) and hence
\[
\int \left| \nabla \psi \right|^2 r dr \sim \int \frac{dr}{r} = \infty
\] (40)
Therefore, in all cases, for any potential, there is a violation of the virial theorem by the irregular solution. This, we believe, settles controversies on the choice of boundary conditions at the origin in a paper on the number of bound states in one and two space dimensions[7].

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