conditions for positive definiteness

1. Mathematisches Institut, LMU München
Theresienstrasse 39, 80333 München, Germany

hainzl@rz.mathematik.uni-muenchen.de

2. Institut für Theoretische Physik,
Universität Wien
Boltzmanngasse 5, A-1090 Vienna,
Austria
rseiring@ap.univie.ac.at

July 12, 2001

Abstract

We present a generalization of the Fefferman-de la Llave decomposition of the Coulomb potential to quite arbitrary radial functions V on $\mathbb{R}^n$ going to zero at infinity. As a byproduct, we obtain conditions for positive definiteness of V, thereby improving results of Askey.

For the description of physical systems interacting with Coulomb forces, the Fefferman-de la Llave decomposition [1] of the Coulomb potential has proved very useful. It states that for $x \in \mathbb{R}^3$

$$\frac{1}{|x|} = \frac{1}{\pi} \int_0^\infty dr \frac{1}{r^5} \chi_r * \chi_r(x),$$

where $\chi_r = \Theta(r - |x|)$ is the characteristic function of a ball of radius r centered at the origin, and $*$ denotes convolution on $\mathbb{R}^3$. Except for the constant $1/\pi$, it is easily checked that (**??**) holds true, since the right hand side is a radial, homogeneous function of order -1. However, for a general function V on $\mathbb{R}^n$, it is not known whether a decomposition of the form (**??**) with a general weight function $g(r)$ replacing $1/r^5$ exists, except for the case $n = 1$ [2].

We show that this is indeed the case, provided some decrease and regularity properties of V are satisfied. Our main result, stated in Theorem 1 below, gives this decomposition, with a weight $g(r)$ that is related to the $[n/2]+2$'th derivative of V. Here $[\cdot]$ denotes the Gauß bracket, i.e., $[m] = \max\{n \in \mathbb{N}_0, n \leq m\}$.

As a byproduct, we see from this decomposition that a function V is positive definite, if the corresponding weight function $g(r)$ is positive. This gives conditions on V which are less restrictive than the ones obtained before by Askey [3].

The decomposition (**??**) may especially be of interest in generalizing results so far only applicable to the Coulomb potential, for instance estimating the "indirect part" of the interaction energy in an N-particle quantum system, as done in the Coulomb case in [4], respectively estimating the validity of Hartree-Fock approximations (see [5] and [6]).

Our main result is the following:

[1] Marie Curie Fellow

1. THEOREM. *Let $V:\mathbb{R}^n\to\mathbb{R}$ be a radial function that is $[n/2]+2$ times differentiable away from $x=0$. For $m\in\mathbb{N}_0$ denote $V^{(m)}(|x|)=d^m/d|x|^m$ V(x).$Assume further that \lim_{|x|\to\infty}|x|^m$ $V^{(m)}(|x|)=0$ for all $0\le m\le[n/2]+1$. Let $\chi_r(x)=\Theta(r-|x|)$, and $n\ge 2$. Then*

$$V(x)=\int_0^\infty dr g(r)\chi_{r/2}*\chi_{r/2}(x),$$

where

$$g(r)=(-1)^{[n/2]}\frac{}{\Gamma(\frac{n-1}{2})\frac{2}{(\pi}}$$
$$r^2)^{(n-1)/2}\left(\int_r^\infty ds V^{([n/2]+2)}(s)\right.$$
$$\left(\frac{d}{ds}\right)^{n-1-[n/2]}s(s^2-r^2)^{\frac{1}{2}(n-3)}$$
$$+\ \delta_{\mathrm{odd}}V^{([n/2]+2)}(r)r$$
$$\left.(2r)^{\frac{1}{2}(n-3)}\Gamma(\tfrac{n-1}{2})\right),$$

(1)

and $\delta_{\mathrm{odd}}=1$ for n odd, $\delta_{\mathrm{odd}}=0$ for n even.

Note the $r/2$ in (**??**), which is chosen for convenience.

Proof. Elementary considerations show that

$$\chi_{r/2}*\chi_{r/2}(x)=\frac{\frac{1}{\Gamma(\frac{n+1}{2})}(}{\pi 4^{(n-1)/2}\int_{|x|}^r dy(r^2-y^2)^{\frac{1}{2}(n-1)}}$$

for $|x|\le r$, and 0 otherwise. Therefore we can write

$$\frac{\genfrac{}{}{0pt}{}{(}{(-1)^{[n/2]}\frac{}{\Gamma(\frac{n-1}{2})\Gamma(\frac{n+1}{2})}}}{12^{n-2-1}\int_0^\infty dr g(r)}$$
$$\chi_{r/2}*\chi_{r/2}(x)=$$
$$\int_{|x|}^\infty dr$$

$$1\frac{\overline{r^{n-1}\int_r^\infty ds V^{([n/2]+2)}(s)(}}{dds^{n-1-[n/2]}s(s^2-r^2)^{\frac{1}{2}(n-3)}\int_{|x|}^r dy}$$

$(\mathrm{r}^2-y^2)^{\frac{1}{2}(n-1)}$

$+\ \delta_{\mathrm{odd}}\int_{|x|}^\infty dr$

$1\frac{}{r^{n-1}V^{([n/2]+2)}(r)r(2r)^{\frac{1}{2}(n-3)}}$

$\Gamma(\frac{n-1}{2})\int_{|x|}^r dy(r^2-y^2)^{\frac{1}{2}(n-1)}.$

Using the fact that

$$\frac{\left(\frac{d}{ds}\right)^{n-1-[n/2]}\int_y^s dr}{1r^{n-1}(r^2-y^2)^{\frac{1}{2}(n-1)}s(s^2-r^2)^{\frac{1}{2}(n-3)}=}$$

$\int_y^s dr\frac{1}{r^{n-1}}(r^2-y^2)^{\frac{1}{2}(n-1)}$

$\left(\frac{d}{ds}\right)^{n-1-[n/2]}s(s^2-r^2)^{\frac{1}{2}(n-3)}$

$+\ \delta_{\mathrm{odd}}\ \frac{1}{s^{n-1}}(s^2-y^2)^{\frac{1}{2}(n-1)}s$

$(2\mathrm{s})^{\frac{1}{2}(n-3)}\Gamma(\frac{n-1}{2}),$

we can change the order of integration to get

(

$$(\text{-}1)^{[n/2]}\frac{\overline{\Gamma(\frac{n-1}{2})\Gamma(\frac{n+1}{2})}}{12^{n-2-1}\int_0^\infty dr g(r)}$$

$\chi_{r/2}*\chi_{r/2}(x)=$

$\int_{|x|}^\infty ds$

$$\frac{\mathrm{V}^{([n/2]+2)}(s)\int_{|x|}^s dy\ (}{dds^{n-1-[n/2]}\int_y^s dr\frac{1}{r^{n-1}}}$$

$\mathrm{s}(\mathrm{s}^2-r^2)^{\frac{1}{2}(n-3)}$

$(\mathrm{r}^2-y^2)^{\frac{1}{2}(n-1)}.$

Now

$\int_y^s dr\frac{1}{r^{n-1}}(s^2-r^2)^{\frac{1}{2}(n-3)}$

$(\mathrm{r}^2 - y^2)^{\frac{1}{2}(n-1)} = \Gamma(\frac{n-1}{2})$
$\Gamma(\frac{n+1}{2})2^{n-2}(s-y)^{n-1}\overline{s\Gamma(n),}$

and therefore

$\int_0^\infty dr g(r)\chi_{r/2} * \chi_{r/2}(x) =$
$\overline{(-1)^{[n/2]}\Gamma([n/2]+2)\int_{|x|}^\infty ds}$
$\mathrm{V}^{([n/2]+2)}(s)(s-|x|)^{[n/2]+1} = V(x),$

where we integrated by parts, using the demanded decrease properties of $|x|^m V^{(m)}(|x|)$. □

2. REMARK. For $n = 1$, (**??**) holds with $g(r) = V''(r)$ [2].

3. REMARK. If $V(x)$ is $n+1$ times differentiable away from $x = 0$, we can use partial integration to write $g(r)$ in the more compact form

$\mathrm{r}^2)^{(n-1)/2}\int_r^\infty ds V^{(n+1)}(s)s$
$(\mathrm{s}^2 - r^2)^{(n-3)/2}.$

For simplicity, we have restricted ourselves to formulating Theorem 1 for differentiable functions only, but as is obvious from the proof, (1) and (**??**) hold for a more general class of potentials, if the derivatives are interpreted in the sense of distributions.

4. EXAMPLE. For the Coulomb potential $V(x) = 1/|x|$, we have

$\mathrm{g(r)=1}\overline{2\frac{\Gamma(n+2)}{\Gamma(n/2+1)}\frac{\pi^{1-n/2}}{r^{n+2}}}.$

The decomposition (**??**) provides conditions for positive definiteness of V. Since $\chi_r * \chi_r(x)$ is obviously positive definite (as a function of x), any V with a positive weight function $g(r)$ is positive definite. This is the content of the following corollary:

5. COROLLARY. *If $g(r) \geq 0$, then $V(x)$ is positive definite.*

It is easy to see that

$\left(\frac{d}{ds}\right)^{n-1-[n/2]} s(s^2 - r^2)^{\frac{1}{2}(n-3)} \geq$
$0 \quad$ for $\mathrm{s} \geq r,$

and therefore positivity of $(-1)^{[n/2]}V^{([n/2]+2)}$ implies
that $V(x)$ is positive definite. Moreover, one needs only
slightly less regularity assumptions on V, and can use Theorem
1 to prove the following theorem, which was also proved
before by Askey [3], who deduces it from certain positivity properties of
Bessel functions proven in [7] and [8].

6. THEOREM. *If $V(x)$ is $[n/2]$ times differentiable away from $x = 0$,
$\lim_{|x|\to\infty} V(x) = 0$ and $(-1)^{[n/2]}V^{([n/2])}(r)$ is
convex for $r > 0$, then $V(x)$ is positive definite.*

Proof. Convexity of $V^{([n/2])}$ together with the decease of V at infinity implies the decrease properties of $|x|^m V^{(m)}(|x|)$ demanded in Theorem 1. Moreover, $V^{([n/2]+2)}$ defines a positive measure, if the last two derivatives are

interpreted in the sense of distributions, and Theorem 1 holds. Since $g(r) \geq 0$, V is positive definite. □

As one sees from (1) and (**??**), the condition
$g(r) \geq 0$, which is sufficient for positive definiteness of
V, is a weaker assumption than $(-1)^{[n/2]}V^{([n/2]+2)} \geq$
$0.Consider for instance the case$n=3.$Here$

$$g(r)=\frac{2}{\pi r^2\left(V''(r)-rV'''(r)\right)=-\frac{2}{\pi}\left(\right.}$$
$$\overline{V''(r)r'},$$

so a monotone decrease of V''/r (instead of V'') is sufficient
for positive definiteness of V. Analogous considerations apply to all dimensions $n \geq 2$.

Positivity of g might be a useful way of checking positive
definiteness of a function V. However, this condition is of
course not necessary, as the following example shows.

7. EXAMPLE. For $n = 3$, $V(x) = 1/(|x|^2 + 1)$ is positive definite, but the corresponding $g(r)$ is not a positive function.

Acknowledgments: We thank Volker Bach for encouraging the present study, and Michael Loss for providing the references [3, 7, 8]. C. Hainzl has been supported by a Marie Curie Fellowship of the European Community programme "Improving Human Research Potential and the Socio-economic Knowledge Base" under contract number HPMFCT-2000-00660. R. Seiringer acknowledges warm hospitality at the Mathematical Institute, LMU München, where part of this work has been done.

References

[1] C.L. Fefferman and R. de la Llave, *Relativistic stability of matter I*, Revista Matematica Iberoamericana **2**, 119–161 (1986)

[2] C. Hainzl and R. Seiringer, *Bounds on One-Dimensional Exchange Energies with Application to Lowest Landau Band Quantum Mechanics*, Lett. Math. Phys. **55**, 133–142 (2001)

[3] R. Askey, *Refinements of Abel Summability for Jacobi Series*, in: Harmonic Analysis on Homogeneous Spaces, Proc. Symp. in Pure Math. **26**, 335–338 (1973)

[4] E.H. Lieb and S. Oxford, *Improved Lower Bound on the Indirect Coulomb Energy*, Int. J. Quant. Chem. **19**, 427–439 (1981)

[5] V. Bach, *Error bound for the Hartree-Fock energy of atoms and molecules*, Commun. Math. Phys. **147**, 527–548 (1992)

[6] G.M. Graf and J.P. Solevej, *A correlation estimate with applications to quantum systems with coulomb interaction*, Rev. Math. Phys. **6**, 977–997 (1994)

[7] R. Askey, *Summability of Jacobi Series*, Trans. Amer. Math. Soc. **179**, 71–84 (1973)

[8] J.L. Fields and M.E. Ismail, *On the Positivity of some ${}_1F_2$'s*, SIAM J. Math. Anal. **6**, 551–559 (1975)