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**Autor:** Bargmann, V.  
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## Note on Some Integral Inequalities

by V. Bargmann

Joseph Henry Laboratories, Princeton University, Princeton,  
New Jersey, USA

(22. II. 72)

To M. Fierz on his sixtieth birthday.

*Abstract.* Inequalities are derived for certain integrals which have the mathematical structure of quantum mechanical expectation values.

### Introduction

This note deals with certain integrals which have the mathematical structure of quantum mechanical expectation values (but in  $n$  instead of three dimensions), namely,

$$I_\mu(\psi) = \int_{R^n} r^\mu |\psi(x)|^2 d^n x, \quad K(\psi) = \int_{R^n} |\nabla \psi|^2 d^n x. \quad (1)$$

Here  $x = (x_1, \dots, x_n)$  is a point in the real  $n$ -dimensional Euclidean space  $R^n$  ( $n \geq 2$ ), and  $r$  its distance from the origin;  $\psi(x)$  is a square integrable, sufficiently well behaved (complex valued) function on  $R^n$ ,  $\nabla \psi$  the gradient of  $\psi$ , and  $|\nabla \psi|^2 = \sum_{j=1}^n |\partial \psi / \partial x_j|^2$ . Finally, the exponent  $\mu$  is real.

We are concerned with a family of inequalities between the various  $I_\mu$  and  $K$ , of which the uncertainty relation is a special case. In section I the functions  $\psi$  are not restricted by any symmetry conditions, and the general inequalities  $(C_\mu)$  are stated in section 1.2. For eigenfunctions of the 'angular momentum' the inequalities are strengthened (see section 3.4). These stronger inequalities  $(C'_{\mu,l})$ , in turn, imply the inequalities  $(C_\mu)$ .

It should be added that, to a certain extent, the discussion in section I is merely heuristic because the class of functions to which it applies is not explicitly defined. The missing precise definitions—in the framework of Hilbert space theory—are supplied in Sections 2 and 3.

Remarks on the notation: 1. The complex conjugate of a complex number  $\alpha$  is denoted by  $\bar{\alpha}$ , its real and imaginary parts by  $\operatorname{Re} \alpha$  and  $\operatorname{Im} \alpha$ , respectively. 2. If  $s$  is a positive real number then  $s^{1/2} = \sqrt{s}$  always denotes its positive square root. 3. The inner product of two  $n$ -component vectors  $a, b$  is denoted by  $a \cdot b = (\sum_{j=1}^n a_j b_j)$ ,  $a^2$  stands for  $a \cdot a$ , and  $|a| = (\sum_j |a_j|^2)^{1/2}$ . 4. In  $n$ -dimensional integrals we write  $d^n x$  for  $dx_1 dx_2 \dots dx_n$  (similarly in momentum space). All  $n$ -dimensional integrals extend over  $R^n$  unless the domain of integration is explicitly indicated.

### 1. The Inequalities for General $\psi$

1.1. We start with an argument which is familiar from the proof of uncertainty relations. Let  $A, B$  be two fixed operators (not necessarily self-adjoint),  $\psi(x)$  a function

on  $R^n$  for which  $A\psi$  and  $B\psi$  are defined and square integrable, and  $\lambda$  a real constant. Then

$$0 \leq \Phi(\lambda) = \|B\psi - i\lambda A\psi\|^2 = \eta_0 \lambda^2 - 2\eta_1 \lambda + \eta_2. \quad (2)$$

The real coefficients  $\eta_k$ , which depend on  $\psi$ , are given by

$$\eta_0 = \|A\psi\|^2, \quad \eta_2 = \|B\psi\|^2 \quad (2a)$$

$$\eta_1 = \frac{1}{2}i\{(B\psi, A\psi) - (A\psi, B\psi)\} = \text{Im}(A\psi, B\psi). \quad (2b)$$

We explicitly assume that  $\eta_0 > 0$ . Then

$$\Phi(\lambda) = \eta_0 (\lambda - \eta_1/\eta_0)^2 + \eta_0^{-1} \zeta \quad (3)$$

$$\zeta = \eta_0 \Phi(\eta_1/\eta_0) = \eta_0 \eta_2 - \eta_1^2 \geq 0$$

Note that  $\Phi(\lambda) = 0$  if and only if  $B\psi = i\lambda A\psi$ . The inequality to be proved follows from (3), namely,

$$\eta_1^2 \leq \eta_0 \eta_2. \quad (4)$$

Equality holds if and only if, for a suitable  $\lambda_0$ ,  $\Phi(\lambda_0) = 0$ , so that  $B\psi = i\lambda_0 A\psi$ , and, by (3)

$$\eta_1 = \lambda_0 \eta_0, \quad \eta_2 = \lambda_0^2 \eta_0. \quad (4a)$$

1.2. Choose now

$$A\psi = r^{\mu+1} \psi, \quad B\psi = -ir^{-1} x \cdot \nabla \psi$$

where  $\mu$  is a real exponent  $\geq -2$  (and  $> -2$  for  $n = 2$ ). We find

$$\begin{aligned} \eta_1 &= -\frac{1}{2} \int \{r^\mu x \cdot (\bar{\psi} \nabla \psi + \psi \nabla \bar{\psi})\} d^n x \\ &= -\frac{1}{2} \int \nabla \cdot (r^\mu x \bar{\psi} \psi) d^n x + \frac{1}{2} \int \bar{\psi} \psi (\nabla \cdot r^\mu x) d^n x. \end{aligned}$$

Assume that the first integral in the last equation vanishes, i.e., that the corresponding surface integral may be neglected. (It suffices that  $\psi$  stays bounded near the origin and vanishes fast enough at infinity.) We then obtain

$$\eta_1 = \frac{1}{2}(n + \mu) I_\mu(\psi)$$

since  $\nabla \cdot (r^\mu x) = (n + \mu)r^\mu$ . Furthermore,

$$\eta_0 = I_{2\mu+2}(\psi), \quad \eta_2 = \int |r^{-1} x \cdot \nabla \psi|^2 d^n x.$$

Clearly,  $|r^{-1} x \cdot \nabla \psi|^2 \leq |\nabla \psi|^2$ . Thus

$$\eta_2 \leq K(\psi) = \int |\nabla \psi|^2 d^n x, \quad (5)$$

and  $\eta_2 = K$  if and only if  $\psi$  is a function of  $r$  only.

From (4) and (5) we obtain now the desired inequality

$$(C_\mu) \quad (\frac{1}{2}(n + \mu) I_\mu(\psi))^2 \leq I_{2\mu+2}(\psi) K(\psi)$$

*The cases of equality.* Equality holds in  $(C_\mu)$  for a non-vanishing  $\psi$  if and only if  $\psi(x) = f(r)$  (by (5)) and  $B\psi = -if'(r) = i\lambda A\psi$ , where  $\lambda = \eta_1/\eta_0 > 0$ . Hence  $f' = -\lambda r^{\mu+1}f$ , and if  $\mu + 2 > 0$  then  $f(r) = cf_{\mu,\lambda}(r)$ ,

$$f_{\mu,\lambda}(r) = \exp\{-\lambda(\mu+2)^{-1}r^{\mu+2}\} \quad (\mu+2 > 0) \quad (6)$$

$$I_{2\mu+2}(\psi) : \frac{1}{2}(n+\mu)I_\mu(\psi) : K(\psi) = 1 : \lambda : \lambda^2. \quad (6a)$$

The inequality  $(C_{-2})$  degenerates into a triviality if  $n = 2$ . Even for  $n \geq 3$  equality never holds (with  $\psi \neq 0$ ) because  $f' = -\lambda r^{-1}f$  has the solution  $f = cr^{-\lambda}$ , which leads to diverging integrals  $I_\mu$  and  $K$ . (See, however, the Appendix.)

1.3. The three cases  $\mu = 0, -1, -2$  deserve to be mentioned because in these cases—apart from the normalization integral  $I_0$ —only one  $I_\mu$  appears in  $(C_\mu)$ . Thus

$$(C_0) \quad (\frac{1}{2}nI_0(\psi))^2 \leq I_2(\psi)K(\psi)$$

$$(C_{-1}) \quad (\frac{1}{2}(n-1)I_{-1}(\psi))^2 \leq I_0(\psi)K(\psi)$$

$$(C_{-2}) \quad (\frac{1}{2}(n-2))^2 I_{-2}(\psi) \leq K(\psi)$$

$(C_0)$  may be considered a form of the uncertainty relation, and  $(C_{-2})$  has long been known (specifically, for  $n = 3$ ) [1].

$(C_{-1})$  has an immediate quantum mechanical application. Let

$$H = \frac{p^2}{2m} - \frac{Ze^2}{r} \quad (7)$$

be the Hamiltonian of a hydrogen-like atom (in  $n$  spatial dimensions!). For a non-vanishing  $\psi$

$$\langle H \rangle_\psi = \frac{\langle \psi, H\psi \rangle}{\langle \psi, \psi \rangle} = \frac{\hbar^2}{2m} \frac{K(\psi)}{I_0(\psi)} - Ze^2 \frac{I_{-1}(\psi)}{I_0(\psi)}$$

is its expectation value, and the minimum of  $\langle H \rangle_\psi$  determines the ground state. Introduce  $\rho = \nu I_{-1}/I_0$ , with  $\nu = \frac{1}{2}(n-1)$ . By  $(C_{-1})$ ,  $K/I_0 \geq \rho^2$ , hence

$$\langle H \rangle_\psi \geq a\rho^2 - 2b\rho = a\left(\rho - \frac{b}{a}\right)^2 - \frac{b^2}{a} \geq -\frac{b^2}{a}$$

with  $a = \hbar^2/2m$ ,  $b = Ze^2/2\nu$ . The minimum,  $-b^2/a$ , is reached for the wave function  $f_{-1,\lambda_0}$  with  $\lambda_0 = b/a$  (by (6) and (6a)). Thus the ground state has the energy  $E = -\frac{1}{2}[(Ze^2)^2 m]/\nu^2 \hbar^2$  and the wave function  $e^{-r/r_0}$ , where  $r_0 = a/b = (\nu \hbar^2)/(Ze^2 m)$ . (In three dimensions, with  $\nu = 1$ , one obtains of course the familiar expressions.)

## 2. Definition of $I_\mu$ , $I_{\mu,l}$ , $K$ and $K_l$ in Hilbert Space

2.1. We turn now to a more precise definition of the admissible functions  $\psi$ , and of the integrals  $I_\mu$  and  $K$ .

First of all, every  $\psi(x)$  is required to belong to the Hilbert space  $\mathfrak{H}(=L^2(R^n))$  of square integrable functions. Then its Fourier transform  $\hat{\psi}(k)$  also belongs to  $\mathfrak{H}$ , and  $\|\hat{\psi}\| = \|\psi\|$ .

If  $I_\mu(\psi) < \infty$  (see equation (1)) we say that  $\psi$  belongs to  $\mathfrak{D}_\mu$ , the domain of  $I_\mu$  (or equivalently, the domain of the operator ‘multiplication by  $r^{\mu/2}$ ’). Clearly,  $\mathfrak{D}_0 = \mathfrak{H}$ .

The crucial point is the proper definition of  $K$ . This is given in terms of  $\hat{\psi}(k)$ , i.e., in momentum space [2]:

$$K(\psi) = \int k^2 |\hat{\psi}(k)|^2 d^n k. \quad (8)$$

If  $K(\psi) < \infty$  then  $\psi$  is said to belong to  $\mathfrak{D}_K$ .  $\mathfrak{D}_\mu$  and  $\mathfrak{D}_K$  are linear manifolds which are dense in  $\mathfrak{H}$ .

**2.2. The Set  $\mathfrak{H}^0$ .** Following Kato [3] we introduce the set  $\mathfrak{H}^0$  of all finite linear combinations of Hermite functions, or, equivalently, of all functions  $\psi$  of the form

$$\psi(x) = p(x) e^{-r^2/2}$$

where  $p$  is any polynomial.  $\mathfrak{H}^0$  has the following extremely useful properties. i)  $\mathfrak{H}^0$  is dense in  $\mathfrak{H}$ ; ii) The Fourier transform maps  $\mathfrak{H}^0$  onto itself; iii)  $\mathfrak{H}^0 \subset \mathfrak{D}_K$ , and  $\mathfrak{H}^0 \subset \mathfrak{D}_\mu$  if  $n + \mu > 0$ .

In addition,  $\mathfrak{H}^0$  may be applied to characterize the domain  $\mathfrak{D}_K$ . In fact,  $\psi$  belongs to  $\mathfrak{D}_K$  if and only if there exists a sequence  $\{\phi_i\} \subset \mathfrak{H}^0$  such that

$$\lim_{i \rightarrow \infty} \|\psi - \phi_i\| = 0 \quad (1) \quad \lim_{\substack{i \rightarrow \infty \\ j \rightarrow \infty}} K(\phi_i - \phi_j) = 0. \quad (2)$$

Then  $K(\psi) = \lim_i K(\phi_i)$ , and  $\lim_i K(\psi - \phi_i) = 0$ .

**2.3. The Subspaces  $\mathfrak{H}_{lt}$  and  $\mathfrak{H}_l$ .** The decomposition of a function  $\psi \in \mathfrak{H}$  into eigenfunctions of the 'angular momentum' in  $n$  dimensions will be defined in terms of harmonic polynomials. A harmonic polynomial of order  $l$  is a homogeneous polynomial  $Z_l$  of order  $l$  which satisfies the Laplace equation, so that

$$x \cdot \nabla Z_l = l Z_l; \quad \Delta Z_l = 0. \quad (9)$$

In terms of standard spherical harmonics  $Y_l$  (defined for points on the unit sphere)  $Z_l(x) = r^l Y_l(r^{-1}x)$ . Among the harmonic polynomials of order  $l$  we may choose an orthonormal basis  $Z_{lt}$ , say, such that

$$\int_{|x|=1} \overline{Z_{lt}(x)} Z_{lt'}(x) d\sigma(x) = \delta_{tt'} \quad (1 \leq t, t' \leq s_l)$$

where  $d\sigma(x)$  is the Euclidean measure on the unit sphere, and  $s_l$  is the number of linearly independent harmonic polynomials of order  $l$ . (Clearly,  $s_0 = 1$ , and  $Z_{01} = \omega_n^{-1/2}$ , where  $\omega_n$  is the area of the unit sphere.) Harmonic polynomials of different orders are of course orthogonal.

The Hilbert space  $\mathfrak{H}$  may be decomposed into the direct sum of pairwise orthogonal subspaces  $\mathfrak{H}_{lt}$ . The elements of  $\mathfrak{H}_{lt}$  are square integrable functions of the form  $\psi(x) = f(r) Z_{lt}(x)$ . Again the Fourier transform maps  $\mathfrak{H}_{lt}$  into itself. For two elements  $\psi_j = f_j Z_{lt}$  of  $\mathfrak{H}_{lt}$  one finds  $(\psi_1, \psi_2) = (f_1, f_2)_l$  where

$$(f_1, f_2)_l = \int_0^\infty \overline{f_1(r)} f_2(r) r^{\beta_l} dr, \quad \beta_l = n - 1 + 2l \quad (10)$$

and in particular  $(\psi, \psi) = (f, f)_l$ .

Thus the functions  $f(r)$  corresponding to the elements  $\psi$  of  $\mathfrak{H}_{lt}$  form a Hilbert space  $\mathfrak{M}_l$  based on the inner product (10), and  $f \in \mathfrak{M}_l$  if and only if  $f$  is measurable and  $(f, f)_l < \infty$ . As usual we set  $\|f\|_l = \sqrt{(f, f)_l}$ .

In  $\mathfrak{H}$  we introduce the projections  $E_{lt}$  on  $\mathfrak{H}_{lt}$ . Thus  $(E_{lt}\psi)(x) = f_{lt}(r)Z_{lt}(x)$ , and for  $f_{lt}$  one finds the integral representation

$$f_{lt}(r) = r^{-\beta_l} \int_{|x|=r} \overline{Z_{lt}(x)} \psi(x) d\sigma(x)$$

where  $d\sigma(x)$  is the Euclidean measure on the sphere  $|x|=r$ , and the integral is defined for almost all  $r$ .

For fixed  $l$  we introduce  $\mathfrak{H}_l = \bigoplus_{t=1}^{s_l} \mathfrak{H}_{lt}$  and the corresponding projection  $E_l = \sum_{t=1}^{s_l} E_{lt}$ . An element  $\psi$  of  $\mathfrak{H}_l$  has the form  $\psi(x) = \sum_t f_{lt}(r)Z_{lt}(x)$ . Note that  $\mathfrak{H}_l$  and  $E_l$  are independent of the choice of the orthonormal basis  $Z_{lt}$ .

Lastly we relate  $\mathfrak{H}_{lt}$  to the set  $\mathfrak{H}^0$  introduced in section 2.2. Obviously  $E_{lt}\mathfrak{H}^0$  is dense in  $\mathfrak{H}_{lt}$ , and it is easily shown that the elements of  $E_{lt}\mathfrak{H}^0$  are functions of the form

$$q(x)Z_{lt}(x)e^{-r^2/2} \quad (11)$$

where  $q$  is a polynomial in  $r^2$ .

2.4. *The Forms  $I_{\mu,l}$ .* If  $\psi$  belongs to  $\mathfrak{D}_\mu$ , so does every  $E_{lt}\psi$ , and

$$I_\mu(\psi) = \sum_{l,t} I_\mu(E_{lt}\psi).$$

$I_\mu(E_{lt}\psi)$ , in turn, may be expressed as  $I_{\mu,l}(f_{lt})$ , where

$$I_{\mu,l}(f) = \int_0^\infty |f(r)|^2 r^{\beta_l + \mu} dr = (r^{\mu/2} f, r^{\mu/2} f)_l. \quad (12)$$

We say that a function in  $\mathfrak{M}_l$  belongs to  $\mathfrak{D}_{\mu,l}$  if  $I_{\mu,l}(f) < \infty$ .

2.5. *The Forms  $K_l$ .* As long as we express  $K(\psi)$  in momentum space the results are quite similar. If  $\psi$  belongs to  $\mathfrak{D}_K$  so does  $E_{lt}\psi$ , and

$$K(\psi) = \sum_{l,t} K(E_{lt}\psi).$$

In order to translate this into the language of configuration space we use the procedure outlined at the end of section 2.2. If  $\psi(x) (= f(r)Z_{lt}(x))$  belongs to  $\mathfrak{H}_{lt}$  the approximating sequence  $\phi_i$  may also be chosen in  $\mathfrak{H}_{lt}$  such that  $\phi_i(x) = u_i(r)Z_{lt}(x)$ , and  $u_i$  (by eq. (11)) has the form  $q \cdot e^{-r^2/2}$ . Thus

$$\|\psi - \phi_i\| = \|f - u_i\|_l.$$

Set  $\phi = \phi_i - \phi_j = u_i Z_{lt}(u(r) = u_i(r) - u_j(r))$ . Then, by equation (8),  $K(\phi) = (\hat{\phi}, k^2 \hat{\phi}) = (\phi, -\Delta \phi)$  since  $k^2 \hat{\phi}$  is the Fourier transform of  $-\Delta \phi$ . In view of equation (9),  $-\Delta \phi = v Z_{lt}$ , where  $v(r) = -u''(r) - \beta_l r^{-1} u'(r)$ . Hence  $K(\phi) = (u, v)_l$  (see (10)), i.e.

$$K(\phi) = - \int_0^\infty \frac{d}{dr} (u u' r^{\beta_l}) dr + \int_0^\infty |u'|^2 r^{\beta_l} dr.$$

Since the first integral vanishes,  $K(\phi) = \|u'\|_l^2$ . For the approximating sequence we find therefore

$$\lim_{i \rightarrow \infty} \|f - u_i\|_l = 0, \quad \lim_{\substack{i \rightarrow \infty \\ j \rightarrow \infty}} \|u'_i - u'_j\|_l = 0, \quad K(\psi) = \lim_i \|u'_i\|_l^2.$$

A closer analysis of these relations shows that a function  $\psi(x) = f(r) Z_{lt}(x)$  in  $\mathfrak{H}_{lt}$  belongs to  $\mathfrak{D}_K$  if and only if  $f$  satisfies the following conditions:  $f \in \mathfrak{M}_l$ , and there exists a function  $g \in \mathfrak{M}_l$  such that

$$f(r_2) - f(r_1) = \int_{r_1}^{r_2} g(r) dr \quad (0 < r_1 < r_2 < \infty) \quad (13)$$

(and hence  $g(r) = f'(r)$  almost everywhere) [4]. Then

$$K(\psi) = K_l(f) = \int_0^\infty |f'(r)|^2 r^{\beta_l} dr = (f', f')_l. \quad (13a)$$

A function  $f$  satisfying these conditions will be said to belong to  $\mathfrak{D}_{K,l}$ .

### 3. Inequalities for the Functions in $\mathfrak{H}_l$

3.1. *The Inequalities for the Functions in  $\mathfrak{H}_{lt}$ .* For fixed  $l$  we consider, for the time being, functions  $f$  which belong to  $\mathfrak{D}_{\mu,l}$ ,  $\mathfrak{D}_{2\mu+2,l}$ , and  $\mathfrak{D}_{K,l}$ —and, hence, also to  $\mathfrak{M}_l$  (see sections 2.4 and 2.5). In section 3.2 the requirements on  $f$  will be relaxed. Set

$$\gamma_{\mu,l} = n + 2l + \mu = \beta_l + 1 + \mu. \quad (14)$$

We assume  $\mu \geq -2$  if  $\beta_l \geq 2$ , and  $\mu > -2$  if  $\beta_l = 1$ , so that  $\gamma_{\mu,l} > 0$ . ( $\beta_l = 1$  implies that  $n = 2$ ,  $l = 0$ .)

Consider the integral

$$J_\rho^\sigma = \gamma_{\mu,l} \int_\rho^\sigma |f(r)|^2 r^{\gamma_{\mu,l}-1} dr = \int_\rho^\sigma |f(r)|^2 \frac{d}{dr} (r^{\gamma_{\mu,l}}) dr.$$

Note that  $J_0^\infty = \gamma_{\mu,l} I_{\mu,l}(f) < \infty$ . If  $0 < \rho < \sigma < \infty$  integration by parts yields

$$J_\rho^\sigma = r^{\gamma_{\mu,l}} |f(r)|^2 \Big|_\rho^\sigma - 2 \operatorname{Re} \int_\rho^\sigma (r^{\mu+1} \bar{f}) f' r^{\beta_l} dr.$$

The two integrals in this equation are absolutely convergent on the interval  $(0, \infty)$  since  $r^{\mu/2} f$ ,  $r^{\mu+1} f$ , and  $f'$  belong to  $\mathfrak{M}_l$ . It follows that  $r^{\gamma_{\mu,l}} |f(r)|^2$  tends to limits  $c_\infty$  and  $c_0$ , say, as  $r \rightarrow \infty$  and  $r \rightarrow 0$ . The convergence of  $J_0^\infty$ , however, implies that  $c_\infty = c_0 = 0$ . In the limit  $\rho \rightarrow 0$ ,  $\sigma \rightarrow \infty$  we find therefore

$$\gamma_{\mu,l} I_{\mu,l}(f) = -2 \operatorname{Re} (r^{\mu+1} \bar{f}, f')_l.$$

From Schwarz' inequality we obtain now the desired result

$$(C_{\mu,l}) \quad (\frac{1}{2} \gamma_{\mu,l} I_{\mu,l}(f))^2 \leq I_{2\mu+2,l}(f) K_l(f)$$

*The cases of equality.* For a non-vanishing  $f$  equality in  $C_{\mu,l}$  holds if and only if  $f' = -\lambda r^{\mu+1} f$  with a positive constant  $\lambda$ . If  $\mu > -2$  it follows, as in section 1.2 that  $f = c f_\mu$ , (see equation (6)). This function meets our requirements, and we have

$$I_{2\mu+2,l} : \frac{\gamma_{\mu,l}}{2} I_{\mu,l} : K_l = 1 : \lambda : \lambda^2. \quad (15)$$

If  $\mu = -2$  equality holds only for  $f = 0$  (see the Appendix for further remarks).

3.2. *Relaxations of the conditions on f.* For every real  $\eta$  set  $I_{\eta,l}(f) = I'_{\eta,l}(f) + I''_{\eta,l}(f)$  where

$$I'_{\eta,l}(f) = \int_0^1 |f|^2 r^{\eta+\beta_l} dr, \quad I''_{\eta,l}(f) = \int_1^\infty |f|^2 r^{\eta+\beta_l} dr.$$

Thus if  $\eta < \zeta$  then  $I''_{\eta,l}(f) \leq I''_{\zeta,l}(f)$  and  $I'_{\zeta,l}(f) \leq I'_{\eta,l}(f)$ . Assume now  $\mu > -2$ , so that  $\mu < 2\mu + 2$ . Then

a)  $I''_{\mu,l}(f) \leq I''_{2\mu+2,l}(f)$ , b)  $I'_{2\mu+2,l}(f) \leq I'_{\mu,l}(f)$ .

Every  $f$  is required to belong to  $\mathfrak{M}_l$ , and hence

c)  $I'_{0,l}(f) + I''_{0,l}(f) = I_{0,l}(f) = \|f\|_l^2 < \infty$ .

We need a fourth estimate, viz.,

d) If  $f \in \mathfrak{D}_{K,l}$  and  $\mu > -2$  then  $I'_{\mu}(f) < \infty$ .

Proof of (d). In view of equation (13) we set, for  $r \leq 1$ ,  $f = f_1 - f_2$ , where  $f_1(r) = f(1)$  and  $f_2(r) = \int_r^1 g(\rho) d\rho$ . Now  $I'_{\mu}(f) \leq 2(I'_{\mu}(f_1) + I'_{\mu}(f_2))$  and, by Schwarz' inequality,

$$|f_2(r)| \leq \|g\|_l \int_r^1 \rho^{-\beta_l} d\rho$$

Thus  $I'_{\mu}(f) < \infty$  as is easily checked, q.e.d.

Our conclusions may now be formulated as follows:

- i) If  $\mu \geq 0$  then  $\mathfrak{D}_{2\mu+2,l} \subset \mathfrak{D}_{\mu,l}$ .
- ii) If  $0 > \mu > -1$  then  $\mathfrak{D}_{K,l} \cap \mathfrak{D}_{2\mu+2,l} \subset \mathfrak{D}_{\mu,l}$ .
- iii) If  $-1 \geq \mu > -2$  then  $\mathfrak{D}_{K,l} \subset \mathfrak{D}_{\mu,l} \cap \mathfrak{D}_{2\mu+2,l}$ .

(Ad i). Note that  $I'_{\mu,l} \leq I'_{0,l}$ . Ad iii) Note that here  $I''_{2\mu+2,l} \leq I''_{0,l}$ .

To sum up: *For the inequalities  $(C_{\mu,l})$  to hold it suffices that  $f \in \mathfrak{D}_{K,l} \cap \mathfrak{D}_{2\mu+2,l}$  if  $\mu > -1$  and that  $f \in \mathfrak{D}_{K,l}$  if  $-1 \geq \mu > -2$ .*

3.3. *Remarks on the case  $\mu = -2$ .* The inequality  $(C_{-2,l})$  remains valid—but reduces to a triviality—if  $\beta_l = 1$ . Assume now  $\beta_l \geq 2$ . Then  $(C_{-2,l})$  is equivalent to

$$(C_{-2,l}) \quad (\frac{1}{2}\gamma_{-2,l})^2 I_{-2,l}(f) \leq K_l(f)$$

and it holds whenever  $f \in \mathfrak{D}_{K,l}$ .

In fact, consider the approximating sequence  $\{u_i\}$  described in section 2.5  $(C_{-2,l})$  applies to  $u_i$  and to  $u_i - u_j$  because these functions satisfy the conditions under which  $C_{-2,l}$  has been derived. Hence  $I_{-2,l}(u_i - u_j)$  tends to 0 as  $i, j \rightarrow \infty$ , and one may conclude that  $f \in \mathfrak{D}_{-2,l}$ , that  $I_{-2,l}(f) = \lim_i I_{-2,l}(u_i)$ , and that  $C_{-2,l}$  holds.

3.4. *Functions on  $\mathfrak{H}_l$  ( $l \geq 1$ ).* It is very easy to generalize our results to functions in  $\mathfrak{H}_l$  (see Sec. 2.3). The case  $l = 0$  may be omitted because  $\mathfrak{H}_0 = \mathfrak{H}_{01}$  (see Sec. 2.3) and the functions in  $\mathfrak{H}_{01}$  are covered by the preceding discussion. Consider a non-vanishing  $\psi \in \mathfrak{H}_l$ . It has the form

$$\psi(x) = \sum_{t=1}^{s_l} f_{lt}(r) Z_{lt}(x) \quad (f_{lt} \in \mathfrak{M}_l).$$

Assume that precisely  $s$  functions  $f_{lt}$  are  $\neq 0$  (where  $s \leq s_l$ ) and that the  $Z_{lt}$  are so ordered that  $f_{lt} \neq 0$  if  $t \leq s$ , and  $f_{lt} = 0$  if  $t > s$ .

If  $\psi \in \mathfrak{D}_\mu$  then all  $f_{lt} \in \mathfrak{D}_{\mu,l}$  (see Sec. 2.4), and by  $(C_{\mu,l})$

$$\frac{\gamma_{\mu,l}}{2} I_\mu(\psi) = \sum_{t=1}^s \frac{\gamma_{\mu,l}}{2} I_{\mu,l}(f_{lt}) \leq \sum_{t=1}^s [I_{2\mu+2,l}(f_{lt}) K_l(f_{lt})]^{1/2}.$$

By Schwarz' inequality

$$\frac{\gamma_{\mu,l}}{2} I_\mu(\psi) \leq \left[ \sum_{t=1}^s I_{2\mu+2,l}(f_{lt}) \right]^{1/2} \left[ \sum_{t=1}^s K_l(f_{lt}) \right]^{1/2},$$

hence

$$(C'_{\mu,l}) \quad \left( \frac{1}{2} \gamma_{\mu,l} I_\mu(\psi) \right)^2 \leq I_{2\mu+2}(\psi) K(\psi).$$

For the validity of these inequalities it suffices that  $\psi \in \mathfrak{D}_K \cap \mathfrak{D}_{2\mu+2}$  if  $\mu > -1$  and that  $\psi \in \mathfrak{D}_K$  if  $-1 \geq \mu \geq -2$ . (This follows from the discussion in sections 3.2 and 3.3.)

The cases of equality. Equality holds in  $(C'_{\mu,l})$  if and only if

- a)  $\left( \frac{1}{2} \gamma_{\mu,l} I_{\mu,l}(f_{lt}) \right)^2 = I_{2\mu+2,l}(f_{lt}) K_l(f_{lt}) \quad (t \leq s)$
- b)  $K_l(f_{lt}) = \alpha I_{2\mu+2,l}(f_{lt}) \quad (t \leq s)$

for some positive  $\alpha$ . Now (a) implies that  $f_{lt} = \kappa_t f_{\mu,\lambda_t}$  (see end of section 3.1), that  $\mu > -2$ , and that  $K_l(f_{lt}) = \lambda_t^2 I_{2\mu+2,l}(f_{lt})$  (by eq. (15)). It follows from (b) that  $\lambda_t = \lambda = \sqrt{\alpha}$  for all  $t$ . Thus

$$\psi(x) = \kappa f_{\mu,\lambda}(r) Z_l(x)$$

where  $\kappa = (\sum_t |\kappa_t|^2)^{1/2}$ , and  $Z_l = \sum_t (\kappa_t / \kappa) Z_{lt}$  is a normalized harmonic polynomial of order  $l$ .

The inequality  $(C_{\mu,l})$  may be considered a special case of  $(C'_{\mu,l})$  for functions  $\psi$  in  $\mathfrak{H}_{lt}$ .

3.5. The inequalities  $(C_\mu)$ . Similarly the results of section 1 may be rederived, but now on a firm basis, in particular as far as the cases of equality are concerned. Consider a non-vanishing  $\psi \in \mathfrak{H}$ , and let  $\psi(x) = \sum_{l,t} f_{lt}(r) Z_{lt}(x)$ . We again have (with  $\gamma_{\mu,0} = n + \mu \leq \gamma_{\mu,l}$ )

$$\frac{1}{2} \gamma_{\mu,0} I_\mu(\psi) = \sum_{l,t} \frac{1}{2} \gamma_{\mu,0} I_{\mu,l}(f_{lt}) \leq \sum_{l,t} \frac{1}{2} \gamma_{\mu,l} I_{\mu,l}(f_{lt})$$

and repeating the steps made in section 3.4 we obtain

$$(C_\mu) \quad \left( \frac{1}{2} \gamma_{\mu,0} I_\mu(\psi) \right)^2 \leq I_{2\mu+2}(\psi) K(\psi).$$

For the validity of  $(C_\mu)$  we have the same sufficient conditions that were stated in section 3.4 following the inequalities  $(C'_{\mu,l})$ .

It is easy to dispose of the cases of equality. Since  $\gamma_{\mu,l} = \gamma_{\mu,0} + 2l$  it is clear that equality holds in  $(C_\mu)$  only if all  $f_{lt}$  vanish except  $f_{01}$ , if  $\mu > -2$ , and  $\psi(x) = c f_{\mu,\lambda}(r)$ .

3.6. Lastly one may extend the discussion of the hydrogen Hamiltonian of equation (7) by asking for the minimum of  $\langle H \rangle_\psi$  for  $\psi \in \mathfrak{H}_l$  (and therefore using  $C'_{-1,l}$  instead

of  $C_{-1}$ ). The analysis is virtually unchanged, but in the definition of  $\rho$  one must replace  $\nu = \frac{1}{2}\gamma_{-1,0}$  by  $\nu + l = \frac{1}{2}\gamma_{-1,l}$ . Thus one obtains

$$E = -\frac{1}{2} \frac{(Ze^2)^2 m}{(\nu + l)^2 \hbar^2}$$

for the minimal energy, and  $\psi(x) = ce^{-r/r_l} Z_l(x)$  for the associated wave function, with  $r_l = (\nu + l)\hbar^2/Ze^2$ .

In similar fashion,  $C_0$  and  $C'_{0,l}$  may be applied to the Hamiltonian of the isotropic harmonic oscillator.

#### APPENDIX: FURTHER REMARKS ON THE CASE $\mu = -2$

As was pointed out in the discussion at the end of section 1.2. equality cannot hold in  $(C_{-2,l})$  if  $f \neq 0$ , so that always

$$K_l(f)/I_{-2,l}(f) > (\frac{1}{2}\gamma_{-2,l})^2 \quad (f \neq 0) \quad (16)$$

if  $\gamma_{-2,l} \neq 0$  (i.e.,  $\beta_l > 1$ ) and  $f \in \mathfrak{D}_{K,l}$ . A more precise relation [5], namely,

$$4K_l(f) - (\gamma_{-2,l})^2 I_{-2,l}(f) = \|2f' + \gamma_{-2,l}r^{-1}f\|^2 \quad (16a)$$

may be derived by combining the identity

$$\|2f' + \gamma_{-2,l}r^{-1}f\|_l^2 = 4K_l(f) + 4\gamma_{-2,l} \operatorname{Re}(r^{-1}f, f')_l + (\gamma_{-2,l})^2 I_{-2,l}(f)$$

(see equations (12) and (13a)) with the equation  $\gamma_{-2,l}I_{-2,l}(f) = -2\operatorname{Re}(r^{-1}f, f')_l$  (see the equation preceding  $(C_{-\mu,l})$  in section 3.1). Note that  $2f' + \gamma_{-2,l}r^{-1}f \neq 0$  if  $f \neq 0$  and  $f \in \mathfrak{M}_l$ .

If  $\beta_l > 1$  equality in (16) may be approached with any desired accuracy. Choose, for example,  $f_\tau(r) = \tau^{1/2} \exp(-\frac{1}{2}r^\tau)$ ,  $\tau > 0$ . Then

$$I_{-2,l}(f_\tau) = \Gamma\left(\frac{\gamma_{-2,l}}{\tau}\right); \quad \frac{K_l(f_\tau)}{I_{-2,l}(f_\tau)} = \frac{\gamma_{-2,l}(\gamma_{-2,l} + \tau)}{4}$$

and equality is approached as  $\tau \rightarrow 0$ .

If, however,  $\beta_l = 1$  ( $n = 2, l = 0$ ) then the ratio  $K_0(f)/I_{-2,0}(f)$  may take any positive value, including 0. (For  $\beta_l = 1, K_0(f) < \infty$  no longer implies that  $I_{-2,0}(f) < \infty$ .)

#### REFERENCES

- [1] See, for example, R. COURANT and D. HILBERT, *Methoden der Mathematischen Physik*, 2nd ed. (Berlin 1931), p. 388, eq. (46).
- [2] See T. KATO's classical paper *Fundamental Properties of Hamiltonian Operators of Schrödinger Type*, Trans. Am. Math. Soc. 70, p. 195–211 (1951) (quoted as KATO I) or his book *Perturbation Theory for Linear Operators* (Springer Verlag, Berlin–Heidelberg–New York 1966) (quoted as KATO II), V, 5.2, and VI, 4.2.
- [3] See KATO I or KATO II, p. 300. Our  $\mathfrak{H}^0$  corresponds to the set  $S$  in KATO II.
- [4] In short,  $f \in \mathfrak{M}_l$ ,  $f$  is absolutely continuous, and  $f' \in \mathfrak{M}_l$ .
- [5] See the analogous relation in: *Inequalities*, by G. H. HARDY, J. E. LITTLEWOOD and G. PÓLYA (Cambridge 1952), p. 178, the equation following (7.4.9).