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Note on Some Integral Inequalities

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(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,

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

Here $x = (x_1, \ldots, x_n)$ is a point in the real n-dimensional Euclidean space R^n ($n \geqslant 2$), 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 ψ, and $|\nabla\psi|^2 = \sum_{j=1}^n |\partial\psi/\partial x_j|^2$. Finally, the exponent μ is real.

We are concerned with a family of inequalities between the various I_μ and K, of which the uncertainty relation is a special case. In section I the functions ψ are not restricted by any symmetry conditions, and the general inequalities (C_μ) 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_μ).

It should be added that, to a certain extent, the discussion in section 1 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 α is denoted by $\bar{\alpha}$, its real and imaginary parts by $\mathrm{Re}\,\alpha$ and $\mathrm{Im}\,\alpha$, 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 $dx_1 dx_2 \ldots dx_n$ (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 ψ

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 λ a real constant. Then

$$0 \leqslant \Phi(\lambda) = \|B\psi - i\lambda A\psi\|^2 = \eta_0\lambda^2 - 2\eta_1\lambda + \eta_2. \tag{2}$$

The real coefficients η_k, which depend on ψ, are given by

$$\eta_0 = \|A\psi\|^2, \quad \eta_2 = \|B\psi\|^2 \tag{2a}$$

$$\eta_1 = \tfrac{1}{2}i\{(B\psi, A\psi) - (A\psi, B\psi)\} = \mathrm{Im}\,(A\psi, B\psi). \tag{2b}$$

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

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

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

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

$$\eta_1^2 \leqslant \eta_0\eta_2. \tag{4}$$

Equality holds if and only if, for a suitable λ_0, $\Phi(\lambda_0) = 0$, so that $B\psi = i\lambda_0 A\psi$, and, by (3)

$$\eta_1 = \lambda_0\eta_0, \quad \eta_2 = \lambda_0^2\eta_0. \tag{4a}$$

1.2. Choose now

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

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

$$\eta_1 = -\tfrac{1}{2}\int\{r^\mu x\cdot(\bar{\psi}\nabla\psi + \psi\nabla\bar{\psi})\}d^n x$$

$$= -\tfrac{1}{2}\int\nabla\cdot(r^\mu x\bar{\psi}\psi)d^n x + \tfrac{1}{2}\int\bar{\psi}\psi(\nabla\cdot r^\mu x)d^n x.$$

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

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

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

$$\eta_2 \leqslant K(\psi) = \int|\nabla\psi|^2\,d^n x, \tag{5}$$

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

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

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

The cases of equality. Equality holds in (C_μ) for a non-vanishing ψ 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 $f(r) = cf_{\mu,\lambda}(r)$,

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

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

The inequality (C_{-2}) degenerates into a triviality if $n = 2$. Even for $n \geqslant 3$ 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_μ 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_μ appears in (C_μ). Thus

(C_0) $\quad (\tfrac{1}{2} n I_0(\psi))^2 \leqslant I_2(\psi) K(\psi)$

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

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

(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

$$H = \frac{p^2}{2m} - \frac{Ze^2}{r} \tag{7}$$

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

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

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

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

with $a = \hbar^2/2m$, $b = Ze^2/2\nu$. The minimum, $-b^2/a$, is reached for the wave function f_{-1,λ_0} with $\lambda_0 = b/a$ (by (6) and (6a)). Thus the ground state has the energy $E = -\tfrac{1}{2}[(Ze^2)^2 m]/\nu^2\hbar^2$ 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_μ, $I_{\mu,l}$, K and K_l in Hilbert Space

2.1. We turn now to a more precise definition of the admissible functions ψ, and of the integrals I_μ 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 ψ belongs to $\mathfrak{D}_\mu$, the domain of I_μ (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]:

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

If $K(\psi) < \infty$ then ψ 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 ψ 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, ψ belongs to $\mathfrak{D}_K$ if and only if there exists a sequence $\{\phi_i\} \subset \mathfrak{H}^0$ such that

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

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

$$x \cdot \nabla Z_l = l Z_l; \quad \Delta Z_l = 0. \tag{9}$$

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

$$\int\limits_{|x|=1} \overline{Z_{lt}(x)} Z_{lt'}(x)\, d\sigma(x) = \delta_{tt'}\ (1 \leqslant t, t' \leqslant s_l)$$

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 ω_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

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

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

Thus the functions $f(r)$ corresponding to the elements ψ 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

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

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 $\mathfrak{H}_l = \oplus_{t=1}^{s_l} \mathfrak{H}_{lt}$ and the corresponding projection $E_l = \sum_{t=1}^{s_l} E_{lt}$. An element ψ 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

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

where q is a polynomial in r^2.

2.4. *The Forms* $I_{\mu,l}$. If ψ 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

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

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 ψ 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 ϕ_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 $\phi = \phi_i - \phi_j = uZ_{lt}(u(r) = u_i(r) - u_j(r))$. 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), $-\Delta\phi = vZ_{lt}$, where $v(r) = -u''(r) - \beta_l r^{-1}u'(r)$. Hence $K(\phi) = (u,v)_l$ (see (10)), i.e.

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

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

$$\lim_{i\to\infty} \|f - u_i\|_l = 0, \qquad \lim_{\substack{i\to\infty\\ j\to\infty}} \|u_i' - u_j'\|_l = 0, \qquad K(\psi) = \lim_i \|u_i'\|_l^2.$$

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*

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

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

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

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

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

We assume $\mu \geqslant -2$ if $\beta_l \geqslant 2$, 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_∞ and c_0, say, as $r \to \infty$ and $r \to 0$. The convergence of J_0^∞, however, implies that $c_\infty = c_0 = 0$. In the limit $\rho \to 0$, $\sigma \to \infty$ 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

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

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 λ. 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

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

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 η set $I_{\eta,l}(f) = I'_{\eta,l}(f) + I''_{\eta,l}(f)$ where

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

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

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

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 $r \leqslant 1, f = f_1 - f_2$, where $f_1(r) = f(1)$ and $f_2(r) = \int_r^1 g(\rho) d\rho$. Now $I'_\mu(f) \leqslant 2(I'_\mu(f_1) + I'_\mu(f_2))$ and, by Schwarz' inequality,

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

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

Our conclusions may now be formulated as follows:

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

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

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* $-1 \geqslant \mu > -2$.

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 $\beta_l \geqslant 2$. Then $(C_{-2,l})$ is equivalent to

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

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 $i,j \to \infty$, 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* $\mathfrak{H}_l$ $(l \geqslant 1)$. 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 $s \leqslant s_l$) and that the Z_{lt} are so ordered that $f_{lt} \neq 0$ if $t \leqslant s$, 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 $(C_{\mu,l})$

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

By Schwarz' inequality

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

hence

$$(C'_{\mu,l}) \quad (\tfrac{1}{2}\gamma_{\mu,l} I_\mu(\psi))^2 \leqslant I_{2\mu+2}(\psi) K(\psi).$$

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* $-1 \geqslant \mu \geqslant -2$. (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) $(\tfrac{1}{2}\gamma_{\mu,l} I_{\mu,l}(f_{lt}))^2 = I_{2\mu+2,l}(f_{lt}) K_l(f_{lt}) \quad (t \leqslant s)$

b) $K_l(f_{lt}) = \alpha I_{2\mu+2,l}(f_{lt}) \quad (t \leqslant s)$

for some positive α. 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 ψ in $\mathfrak{H}_{lt}$.

3.5. *The inequalities* (C_μ). 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 $\gamma_{\mu,0} = n + \mu \leqslant \gamma_{\mu,l}$)

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

and repeating the steps made in section **3.4** we obtain

$$(C_\mu) \quad (\tfrac{1}{2}\gamma_{\mu,0} I_\mu(\psi))^2 \leqslant I_{2\mu+2}(\psi) K(\psi).$$

For the validity of (C_μ) 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_μ) 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 ρ 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

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

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

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

may be derived by combining the identity

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

(see equations (12) and (13a)) with the equation $\gamma_{-2,l} I_{-2,l}(f) = -2\,\mathrm{Re}(r^{-1}f, f')_l$ (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

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

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

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).