Problem Sheet 5

Due date: 5 October 2016 16:00

For full credit, you should hand in a tidy and efficiently short presentation of your results and how they come about, in a manner that can be understood and reproduced by your peers. All problems and solutions are for your personal use only. Please do not pass solutions or problems on to incoming or other students who have not taken the course (yet). Noncompliance with these rules is a breach of academic integrity.

Handwritten solutions must be on 5x5 quadrille paper; electronic solutions must be in .pdf format.
I reserve the right to award zero points for any illegible, chaotic or irreproducible section of your homework.

1. Scalar Product for Matrices (5P): The scalar product can come in surprising disguises. Given two arbitrary, quadratic matrices $M$ and $N$ with the same dimensions, which do not have to be symmetric, Hermitean or even diagonalisable. Show: The operation

$$\langle M, N \rangle := \text{tr}[M^\dagger N]$$

defines a scalar product and is positive definite. For the latter, it helps to recall that a matrix consists of rows of column vectors (or vice versa).

2. Rayleigh-Ritz Variational Method (7P): The Hamilton operator of the harmonic oscillator is in appropriate units

$$H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2.$$ 

a) (5P) By varying the parameter $c$ in the trial function

$$\phi_0(x) = \begin{cases} (c^2 - x^2)^2 & \text{for } |x| < c \\ 0 & \text{for } |x| \geq c \end{cases},$$

obtain an upper bound for the ground-state energy and wave-function. Notice that $\phi_0$ is not yet normalised and that it vanishes outside the interval $[-c; c]$, which makes the integrals easier.

b) (2P) Compare to the exact result, also by calculating the “overlap” between the trial and exact wave-function. Interpret the overlap as the amount by which the two wave functions are “aligned” and provide a number for the “angle” between the two wave functions in the abstract space of functions. You may not be able to do the integral exactly.

Please turn over.
3. **Gram-Schmidt Ortho-Normalisation (7P):** We now use the Gram-Schmidt ortho-normalisation procedure familiar from Linear Algebra to construct ortho-normal sets of functions, see e.g. [AW, Sects. 3.1 and 10.3]. While “ortho-normal” has a familiar meaning for vectors, we have to define what we mean by ortho-normal functions. To that end, *define* two functions \( f, g \) in \( n \)-dimensional space as orthogonal to each other when \( \int d^nr \, w(\vec{r}) \, f(\vec{r})^{\dagger} g(\vec{r}) = 0 \), normalised when \( \int d^nr \, w(\vec{r}) \, |f(\vec{r})|^2 = 1 \), where \( w(\vec{r}) \) is a “weight function” which is given, the integration region may be finite or infinite, and “\( ^\dagger \)” denotes complex conjugation. This definition constitutes a functional and is in itself a reasonable extension of the notion of ortho-normal vectors. The Gram-Schmidt ortho-normalisation procedure aims now to construct a **Complete Ortho-Normal Basis** of the space of all function on the integration region, from a set of trial functions. To show that this basis is complete can be lengthy, see the later chapter on Functional Analysis.

The most famous set of trial functions is the set \( \{ x^n, n \in \mathbb{N}_0 \} \) of all non-negative integer powers of \( x \). On the interval \( r \in [-1; 1] \) and with \( w(r) = 1 \), taking this as the “seed” of the Gram-Schmidt procedure leads for example to the **Legendre Polynomials**, see [AW, Example 10.3.1]. Other choices for \( w \) and intervals lead to other complete ortho-normal sets of special functions, which in general are called **Orthogonal Polynomials**.

a) **(5P)** Construct now the first 3 (three) ortho-normal functions for the seed \( \{ x^n \} \) on the positive real half-line, \( r \in [0; \infty[ \), with weight factor \( w(r) = e^{-r} \). These are some of the **Laguerre Polynomials** which appear in the radial solution of the Hydrogen wave-function.

b) **(2P)** After what you have learned about Gram-Schmidt ortho-normalisation, how would you improve your trial wave-function for the Rayleigh-Ritz problem above? An outline of your reasoning is enough, but state the first improvement of the wave-function you would use. Do *not* provide a full-blown calculation.

4. **Group or No Group (3P):** Consider the following sub-sets of the group of invertible, real \( 3 \times 3 \) matrices \( M \in GL(3, \mathbb{R}) \). Do these sets form groups under matrix multiplications? If yes, what is their identity element?

a) **(1P)** The set of matrices which obeys \( M^T = M \).

b) **(2P)** The set of matrices which obeys \( (M)_{ij} = 0 \) for \( i > j \) and whose diagonal elements are all nonzero (“upper-triangular matrices”).

5. **A Group of Functions (8P):** Given the functions below and the operation \( f_i(x) \circ f_j(x) = f_i(f_j(x)) \).

\[
\begin{align*}
&\left\{ f_1(x) = x; \ f_2(x) = 1 - x; \ f_3(x) = \frac{1}{x} \right\}.
\end{align*}
\]

a) **(3P)** Construct the full group operation table of the smallest group which contains these elements. At least three elements must be added to make the whole set of elements a group.

b) **(3P)** Is this group Abelian? Identify the inverse of each group element. Which function serves as the identity element?

c) **(2P)** List *all* proper sub-groups, i.e. all subgroups which are not the identity or the group itself.