Sturmian Basis Functions for the Harmonic Oscillator

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Abstract

We define Sturmian basis functions for the harmonic oscillator and investigate whether recent insights into Sturmians for Coulomb-like potentials can be extended to this important potential. We also treat many body problems such as coupling to a bath of harmonic oscillators. Comments on coupled oscillators and time-dependent potentials are also made.

It is argued that the Sturmian method amounts to a non-perturbative calculation of the energy levels, but the limitations of the method is also pointed out, and the cause of this limitation is found to be related to the divergence of the potential. Thus the divergent nature of the anharmonic potential leads to the Sturmian method being less accurate than in the Coulomb case. We discuss how modified anharmonic oscillator potentials, which are well behaved at infinity, leads to a rapidly converging Sturmian approximation.

1 Introduction

A typical situation in quantum theory is to be faced with a physical potential \( V \) for which one has to solve the corresponding equation of motion, find

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the energies etc. For most realistic potentials it is impossible to find the energies and wave functions analytically, hence one must resort to various approximation or numerical schemes. It is the purpose of this paper to extend one such approximation scheme from Coulomb-like potentials to harmonic and anharmonic oscillators.

The general situation in quantum theory is a system of $N$ particles interacting through some potential $V_0(x_1, ..., x_N)$. The equation of motion is then an equation of the general form

$$(D + V_0 - E)\psi = 0$$

where $D$ is some differential operator of first or second order, $V_0$ is the above-mentioned potential and $E$ is an eigenvalue. Examples are (units where $\hbar = c = 1$)

1. The Dirac equation $D = i\gamma^0 \gamma^\mu \partial_\mu$ (summation over repeated indices implied, $\mu = 0, 1, 2, 3$, $\gamma^\mu$ are the Dirac matrices), $V_0 = v_0(x) + \gamma^0 m$, $v_0(x)$ some potential.

2. The Schrödinger equation $D = \frac{1}{2m} \nabla^2$ where $\nabla^2$ is the Laplace operator in $d$ dimensions.

3. The Klein-Gordon equation where $D = \Box$, the d’Alembertian operator, $V_0 = m^2 + v_0(x)$.

For $N > 1$ we simply have $D = \sum_{i=1}^N D_i$ where $D_i$ is the appropriate operator for the $i$'th particle. Thus all of relativistic as well as non-relativistic quantum mechanics fall into this category (even in curved spacetimes). Usually one finds a complete set of eigenstates corresponding to the different values of $E$, since $D$ is Hermitian these form an orthonormal set. The problem is, however, that for many cases continuous as well as discrete eigenvalues have to be taken into account in order to get a basis for the full Hilbert space. This is for instance the case in the Coulomb potential case already in non-relativistic quantum mechanics, where the continuum eigenstates are needed to get completeness. Consequently, alternatives will have to be found.

Shull and Löwdin, [1], introduced another approach for the Coulomb potential. Their methods were generalised by Rotenberg who also coined the word “Sturmians” for the new basis set, [2]. It has recently been realised that this approach can be even further generalised to handle, e.g., many centre
potentials, [4] as well as relativistic effects, [7] and many-particle systems [6].
It is the purpose of this paper to outline the general theory and to apply it
to other potentials such as harmonic oscillators and variations thereof.
Instead of finding a set of eigenfunctions all corresponding to the same “cou-
ingling constants”, i.e., charges for the Coulomb and Yukawa potentials, \( m\omega^2 \)
for the harmonic oscillator etc., but to different energies as one normally
does, one can take the “dual” approach and fix the energy \( E \) and then allow
the coupling constants to vary. Thus we consider not the original equation
(1) but instead
\[
(D + \beta_n V_0 - E)\psi_n = 0
\]
where \( \beta_n \) is some constant depending on the set \( n \) of quantum numbers.
The solution of this equation gives \( E \) as a function of \( \beta_n \) which can then be
inverted to find \( \beta_n \) as a function of \( E \), assuming we can solve the equation
(2), of course. We will refer to \( \beta_n \) as the effective coupling constant – for
\( V_0 = -Z/r \) it corresponds to scaling the nuclear charge, for \( V_0 = m\omega^2x^2 \) it
 corresponds to scaling the mass and/or the frequency.
The assumed Hermiticity of \( D \) then implies
\[
(\beta_n - \beta_n') \int \psi_n^* V_0 \psi_n dx = 0
\]
i.e., the Sturmian functions satisfy the potential weighted orthogonality rela-
tion
\[
\int \psi_n^* V_0 \psi_n' dx = N_n \delta_{nn'}.
\]
Strictly speaking (3) only implies \( \int \psi_n^* V_0 \psi_n' dx = 0 \) for \( \beta_n \neq \beta_n' \). For sufficiently nice potentials, i.e., potentials without any violent oscillations, such
that the energy \( E \) depends monotonically on the quantum numbers \( n \), the
orthonormality condition (4) follows. An example of a potential which we do
not expect to be able to handle with this approach is \( V_0(x) = \frac{\sin x}{x} \), but potentials \( x^{-1}, x^{-1}e^{-kx}, x^2 \) can be treated this way. It will also be shown later that
the many centre analogues of these potentials also are within reach. Another
subtlety concerns “major” and “minor” quantum numbers in the terminol-
ogy of Aquilanti and Avery, [5]. The coefficients \( \beta_n \) need not depend on all
quantum numbers, those on which it does depend are referred to as “major”
and the remaining ones are then “minor”. For the Coulomb potential, for
instance, \( \beta_n \) only depends on \( n \) and not on the angular momentum quantum
numbers \( l, m \). The orthogonality with respect to the minor quantum

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numbers following from the orthonormality of the spherical harmonics $Y_{lm}$ and the separation of variables, $\psi_n(r, \Omega) = \chi_n(r)Y_{lm}(\Omega)$. For the harmonic oscillator no such subtlety occurs.

To solve the Schrödinger, Klein-Gordon or Dirac equation for some physical potential $V$, we begin by considering Sturmians corresponding to a “base potential” $V_0$ for which we can easily solve the corresponding differential equation to find the basis set. If $V_0$ is sufficiently similar to $V$, the convergence has been found, for the Coulomb and Yukawa potentials, to be very rapid, and, if $E$ is taken to be the actual physical energy the Sturmians will, furthermore, have the right asymptotic behaviour. We will see, however, that this rapid convergence only takes place when the potential (or rather its matrix elements) have sufficiently nice convergence properties themselves.

Equation (4) has far reaching consequences. Consider a new potential $V_0 \rightarrow V = V_0 + V'$, where $V_0$ is some potential for which we can easily find the Sturmians (say, $V_0 \sim r^{-1}$ or $V_0 \sim x^2$).\(^1\) The equation of motion for this new system is then

$$ (D + V_0 + V' - E')\psi = 0 $$

and we can expand $\psi$ on the Sturmians for $V$ as $\psi = \sum_n c_n \psi_n$ to obtain

$$ (D + V_0 + V' - E') \sum_n c_n \psi_n = \sum_n c_n [(1 - \beta_n)V_0 + V' + E - E'] \psi_n $$

upon using (2). From this we get the secular equation by using the potential weighted orthogonality relation. Thus

$$ \sum_n [(1 - \beta_n)N_n \delta_{nn'} + \langle \psi_n'|V'|\psi_n \rangle + (E - E')\langle \psi_n'|\psi_n \rangle] c_n = 0 $$

from which the kinetic energy has disappeared and only the potential $V'$ appears together with the overlap integrals of the Sturmians. It is this feature of Sturmians which is so important. It often implies that one can find $E'$ with very great accuracy from an extremely small basis set, even with just one basis function, $\psi_n$, in which case we have simply

$$ E' = (1 - \beta_n)N_n + \langle \psi_n|V'|\psi_n \rangle $$

\(^1\)Often, when working with Sturmians, one would like to take $V' = V$ to be a physical potential, and only use $V_0$ to find the basis set. We will want to include $V_0$ as part of the physical potential in this paper, however.
giving an explicit formula for $E'$, which when $V'$ is sufficiently close to $V_0$ is a surprisingly good fit, [4, 7]. The reason for this success is to be found in the very construction of Sturmians. By construction, Sturmians take the potential much more into account, and thus contain much more information about the potential. In a sense, Sturmian functions are optimised with respect to the specific features of the given potential, and it is precisely this that lies behind their success in the Coulomb case.

Another consequence of this can be seen if one attempts to use Sturmians as a starting point for a variational calculation. Suppose we know the Sturmians for $V_0$, and now want to use variational theory to estimate the ground state energy of the Hamiltonian $H = D + V_0 + V'$, using the standard formula

$$E_0 \leq \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

with $\psi = \psi_n$, a Sturmian, we get

$$E_0 \leq E + (1 + \beta_n) \frac{\langle \psi_n | V_0 | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle} + \frac{\langle \psi_n | V' | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle}$$

which only concerns the starting potential $V_0$ and the energy $E$ to which the Sturmians correspond. If the Hamiltonian, moreover, is of the form $H = D + V'$, we get

$$E_0 \leq E + \beta_n \frac{\langle \psi_n | V_0 | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle} + \frac{\langle \psi_n | V' | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle}$$

which, in any case, is a rather simple integral to compute, suggesting that Sturmians be a good starting point for variational calculations.

It should be noticed, that one will often assume $E = E'$ to be an allowed energy also of the “perturbed” potential $V = V_0 + V'$ for an appropriate value of the effective couplings $\beta_n$. In this instance (1) can be seen as showing the physical effect of the $\beta_n$ as a kind of screened charge in the Coulomb and Yukawa cases: $(1 - \beta_n)$ measures the “screening”. Now, $\beta_n = 1$ corresponds to an unscaled coupling constant, from $(1 - \beta_n) \propto \langle \psi_n | V' | \psi_n \rangle$ we see that for $E = E'$ to be an allowed energy value also for $V = V_0$, we must fit the coupling constant $\beta_n$ to exactly the right value as given by the perturbation $V'$.

Since the above consideration only used that $D$ was Hermitian, the results
hold for all the abovementioned cases provided we can find effective couplings $\beta_n$ such that $E$ can be held fixed. It is known that such $\beta_n$ exist for the Coulomb, Yukawa potentials both in relativistic (the Dirac equation) and non-relativistic quantum mechanics and also for their many centre analogues. It will similarly be shown that this also holds for the harmonic oscillator. In fact, the following argument seems to suggest that it will always hold. Write the original potential as $V_0(x) = \alpha x$ where $\alpha$ is some constant, the original coupling constant, specifying the strength of the potential, e.g., $\alpha = Z$ for the Coulomb case. Clearly, $E = E(\alpha)$ if $E$ is an allowed energy eigenvalue. If there is no degeneracy, a choice for $\alpha$ and for the set of quantum numbers $n$ uniquely specify the energy $E$, and thus we can invert the relation to find $\alpha$ as a function of $E$ and $n$. If there is degeneracy, the equation $\alpha = \alpha(E, n)$ has more than one solution in the physical range, but this merely mean that more than one set of quantum numbers exists giving the same energy, for each such choice of quantum numbers we get a new solution $\beta_n = \alpha(E, n)$. Another interesting relationship is the momentum space orthonormality relation. Let $\phi_n(k)$ be the Fourier transform of $\psi_n(x)$, this then satisfies

$$ (D^t - E)\phi_n = -\beta_n V_0^t * \phi_n $$

where $D^t, V_0^t$ are Fourier transforms of $D, V_0$ and where $*$ denotes convolution,

$$ V_0^t * \phi_n = \int V_0^t(k - k')\phi_n(k')dk' $$

Multiply by $\phi_n^* \phi_n$ from the left and perform the $k$-integral to arrive at

$$ \int \phi_n^*(D^t - E)\phi_n dk = -\beta_n \int \phi_n^*(V_0^t * \phi_n) dk $$

Now, by the Fourier convolution theorem, $(fg)^t = f^t * g^t$, and Parzival’s formula, $\langle f|g \rangle = \langle f^t | g^t \rangle$, we get

$$ \int \phi_n^t(D^t - E)\phi_n dk = -\beta_n N_n \delta_{nn'} $$

Hence, the momentum space Sturmians satisfy a weighted orthonormality relation where the weighting factor is given by the kinetic part of the equation of motion and not the potential as in $x$-space. For the three operators $D$
mentioned in the beginning, this relation reads

\[
\int \phi'^*_{n'}(\gamma^\nu \gamma^\mu k_{\mu} - E - \gamma^0 m) \phi_n dk = -\beta_n N_n \delta_{nn'}
\]

\[
\int \phi'^*_{n'}(k^2 - 2mE) \phi_n dk = -2m\beta_n N_n \delta_{nn'}
\]

\[
\int \phi'^*_{n'}(k^2 - m^2 - E) \phi_n dk = -\beta_n N_n \delta_{nn'}
\]

for the Dirac, Schrödinger and Klein-Gordon equation respectively. In the non-relativistic case, one will often write \(k_0^2 = -2mE\), which is then positive \((k_0\) real) for bound states and negative \((k_0\) imaginary) for unbound states. In this case, the weighting factor becomes \(k^2 + k_0^2\) which can be interpreted as the length of the momentum vector in \(d + 1\) dimensions. It is this extra dimension which is related to Fock’s famous treatment of the Hydrogen atom where he finds the existence of a \(SO(4)\)-symmetry. This can be generalised to arbitrary dimensions by means of hyperspherical harmonics, [3, 4].

The momentum space relations have other important implications. The equations of motion in momentum space is

\[
(D^t - E)\phi_n(k) = -\beta_n V_0^d \ast \phi_n
\]  

(14)

Define, for simplicity, \(\tilde{\phi}_n = (D^t - E)\phi_n\), then we can write the momentum space orthonormality relation as \(\int \phi_{n'}^* \phi_{n'} dk = -\beta_n N_n \delta_{nn'}\) and the equation of motion as

\[
\tilde{\phi}_n(k) = -\beta_n (V_0^d \ast \phi_n)(k)
\]

\[
= -\beta_n \int V_0^d(k - k') \phi_n(k') dk'
\]

(15)

(16)

Now, make the following Ansatz

\[
V_0^d(k - k') = \sum_n c_n \tilde{\phi}_n(k) \tilde{\phi}_n^*(k')
\]

(17)

Inserting this into (16) we then get

\[
c_n = \frac{N_n}{\beta_n^2}
\]

(18)
i.e.,

\[ V_0'(k - k') = \sum_n \frac{N_n}{\beta_n^2} \phi_n(k) \tilde{\phi}_n(k') \]

(19)

\[ := \sum_n \frac{N_n}{\beta_n^2} D'(k)(D'(k'))^* \phi_n(k) \tilde{\phi}_n(k') \]

(20)

When \( V_0' \) is some function of \( k, k' \), this is a useful summation formula for the momentum space Sturmians. When \( V_0' \) is a differential operator, on the other hand, as happens when \( V_0 = x^\gamma, \gamma > 0 \), then this is a spectral representation of that operator.

It should be emphasised that the coefficients in the above expansion are very simple in the sense that they are the natural quantities related to the basis set, namely the normalisation, the “effective charge” \( \beta_n \), and the kinetic operator (which is then a polynomial in momentum space). This shows more precisely how Sturmians are adapted to the potential.

We will now turn to the specific case of a harmonic oscillator.

\section{The Harmonic Oscillator}

To begin with we work with \( N = 1 \) and in \( d = 1 \) dimension. The potential is \( V_0 = \frac{1}{2}x^2 \) and we solve the equation

\[ \left( -\frac{1}{2m} \frac{d^2}{dx^2} + \frac{1}{2} \beta_n x^2 - E \right) \psi_n = 0 \]

(21)

which is the harmonic oscillator Schrödinger equation with \( m\omega^2 \) replaced by \( \beta_n \). We will henceforth use mass weighted coordinates and put \( m = 1 \), if the mass needs to be reinstated one simply replaces \( x \) by \( \sqrt{mx} \). In this case \( \omega \) in the original harmonic oscillator Hamiltonian has been replaced by \( \beta_n^{1/2} \). The solution of this is clearly

\[ \psi_n(x) = \pi^{-1/4}(n!)^{-1/2}2^{-n/2}H_n((\beta_n)^{1/4})e^{-\frac{1}{2}\beta_n^{1/2}x^2} \]

(22)

where \( n = n \) is a non-negative integer, \( H_n \) is a Hermite polynomial and \( E = \omega(n + \frac{1}{2}) = \sqrt{\beta_n}(n + \frac{1}{2}) \). From this relationship between \( E, n, \beta_n \) we read off

\[ \beta_n = \left( \frac{E}{n + \frac{1}{2}} \right)^2 \]

(23)
which is the promised relationship between the effective coupling, the quantum number and the energy, needed to make the Sturmian machinery work. The effect of scaling the argument by an \( n \)-dependent quantity is to scale all the functions to take values within the same interval. This is illustrated in figure 1.

The orthonormality relation, \( \langle \psi_n | \frac{1}{2} x^2 | \psi_{n'} \rangle = N_n \delta_{nn'} \), then reads

\[
\int H_n(\beta_n^{1/4}x) H_{n'}(\beta_{n'}^{1/4}x) e^{-\frac{1}{2}(\beta_n^{1/2}+\beta_{n'}^{1/2})x^2} x^2 dx = N_n \sqrt{\pi} 2^{n+1} n! \delta_{nn'} \quad (24)
\]

The first few normalisation factors \( N_n \) turn out to be as in table 1, we see that \( N_n \sim E^{-3/2} \) — in general, \( \langle \psi_n | x^k | \psi_{n'} \rangle \sim E^{-(k+1)/2} \) for \( k = 0, 1, 2, ... \). This is easily seen from a simple scaling argument: Perform the scaling \( x \rightarrow \beta_n^{1/4}x \sim E^{1/2}x \) (for the sake of this argument we can ignore the \( n \) dependence), in the integral and the result follows directly.

From table 1 it is clear that

\[
N_n = \frac{(2n+1)^{3/2}}{8 \sqrt{2}} E^{-3/2} = \frac{1}{4} \beta_n^{-3/4} \quad (25)
\]

Notice that the Sturmian orthonormality relation above differs slightly from the usual one in two ways, (1) the Hermite polynomials have different arguments (normally the argument is just \( \sqrt{\omega} x \), irrespective of the value of the quantum number \( n \)), and (2) the appearance of the factor \( x^2 \).

Similarly, the overlap matrix between the first five Sturmians \( T_{nn'} = \int \psi_n^* \psi_{n'} dx \) is

\[
T = E^{-1/2} \begin{pmatrix}
\frac{1}{\sqrt{2}} & 0 & -\frac{1}{3} \sqrt{\frac{5}{3}} & 0 & \frac{12}{25} \sqrt{\frac{5}{7}} \\
0 & \frac{1}{\sqrt{2}} & 0 & -\frac{21}{25} \sqrt{\frac{5}{7}} & 0 \\
-\frac{1}{3} \sqrt{\frac{5}{3}} & 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{132}{343} \sqrt{\frac{5}{7}} \\
0 & -\frac{21}{25} \sqrt{\frac{5}{7}} & 0 & \frac{1}{\sqrt{2}} & 0 \\
\frac{12}{25} \sqrt{\frac{5}{7}} & 0 & -\frac{132}{343} \sqrt{\frac{5}{7}} & 0 & \frac{3}{\sqrt{2}}
\end{pmatrix} \quad (26)
\]

For \( d > 1 \), the energy spectrum is \( E = \omega (n + d/2) \) leading to a very simple modification in the expression linking \( \beta_n \) and \( E \). The wave functions become products of Hermite polynomials and \( \mathbf{n} = (n_1, ..., n_d) \), \( n = n_1 + n_2 + ... + n_d \)

\[
\psi_n = \pi^{-d/4} 2^{-dn/2} \left( \prod_{i=1}^{d} (n_i)! \right)^{-1/2} H_{n_1}(\beta_n^{1/4} x_1) \ldots e^{-\frac{1}{2} \beta_n^{1/2} (x_1^2 + ... x_d^2)} \quad (27)
\]
Note, $\beta_n = \beta_n$ depends only on $n = n_1 + \ldots + n_d$, the “total quantum number”. The case of more than one particle merely corresponds to a harmonic oscillator in $D = dN$ dimensions, where $N$ denotes the number of particles and $d$ the number of spatial dimensions. If the particles have different masses, one have to use mass-weighted coordinates, $x_i \mapsto y_i = \sqrt{m_i}x_i$, but otherwise no modifications are needed. Clearly, all the important features can be found already in the $d = N = 1$ case, for which reason we will stick to this situation in the following unless otherwise stated.

The momentum space formulation of the harmonic oscillator needs the Fourier transform of the Hermite polynomials. It is proven in the appendix that

$$\phi_n(k) = \pi^{-1/4} (n!)^{-1/2} 2^{-n/2} \sqrt{\frac{2\pi}{\beta_n^{1/4}}} \left( 1 + \frac{1}{2} (\beta_n)^{1/4} \right) \times$$

$$H_n(i k (1 + \frac{1}{2} \beta_n^{1/4})^{-1/2} e^{\frac{1}{2} k^2} \beta_n^{-1/2}$$

is the Fourier transform of $\psi_n$. The Hermite polynomials of imaginary arguments appear in this formula, this means that for $n$ even $\phi_n$ is purely real, whereas for $n$ odd it is purely imaginary. The momentum space orthogonality relation then gives the following new relationship between Hermite polynomials

$$\int H_n(i k (1 + \frac{1}{2} \beta_n^{1/4})^{-1/2}) H_n'(i k (1 + \frac{1}{2} \beta_{n'}^{1/4})^{-1/2}) e^{\frac{1}{2} k^2 (\beta_n^{1/2} + \beta_{n'}^{1/2})} (k^2 - 2E) dk$$

$$= -\frac{1}{\sqrt{2\pi}} n! 2^{n+1/2} \beta_n^{5/4} N_n \left( 1 + \frac{1}{2} \beta_n^{1/4} \right)^{-2} \delta_{nn'}$$

a somewhat unexpected result.

### 3 The Anharmonic Oscillator

We now add a new potential $V' = \alpha x^3$ to $V$. We then need to compute the matrix elements of this in the basis of harmonic oscillator Sturmians. We need to compute the matrix $W_{nn'}^{(3)} = \int \psi_n^{*} x^3 \psi_{n'} dx$. For $n, n' = 0, 1, \ldots, 4$ we
get the following explicit result

\[
W^{(3)} = E^{-2} \begin{pmatrix}
0 & \frac{27}{64} & 0 & -\frac{343\sqrt{3}}{2048} & 0 \\
\frac{27}{64} & 0 & \frac{7425\sqrt{2}}{2048} & 0 & -\frac{3159}{512\sqrt{2}} \\
0 & \frac{7425\sqrt{2}}{2048} & 0 & \frac{671425\sqrt{2}}{41472} & 0 \\
-\frac{343\sqrt{3}}{2048} & 0 & \frac{671425\sqrt{2}}{41472} & 0 & \frac{331831169}{4194304} \\
-\frac{3159}{512\sqrt{2}} & 0 & 0 & \frac{331831169}{4194304} & 0
\end{pmatrix}
\] (30)

The secular equation then reads

\[
\operatorname{det}( (1 - \beta_n)N_n \delta_{nn'} + \alpha W^{(3)} ) = 0
\] (31)

By including the first \( N \) Sturmians we get the ground state energies shown in table 2 with \( \alpha = .1 \).

Another version is \( V' = x^4 \), for this case the matrix \( W^{(4)} := \int \psi_n^* x^4 \psi_{n'} dx \) becomes

\[
W^{(4)} = E^{-5/2} \begin{pmatrix}
\frac{3}{16\sqrt{2}} & 0 & \frac{25}{144}\sqrt{\frac{5}{3}} & 0 & -\frac{243}{1000}\sqrt{\frac{3}{5}} \\
0 & \frac{135}{16}\sqrt{\frac{3}{2}} & 0 & \frac{27783}{2000}\sqrt{\frac{3}{5}} & 0 \\
\frac{25}{144}\sqrt{\frac{5}{3}} & 0 & \frac{925}{16}\sqrt{\frac{5}{2}} & 0 & \frac{625725}{9004}\sqrt{\frac{15}{14}} \\
0 & \frac{27783}{2000}\sqrt{\frac{3}{5}} & 0 & \frac{3675}{16}\sqrt{\frac{7}{2}} & 0 \\
-\frac{243}{1000}\sqrt{\frac{5}{3}} & 0 & \frac{625725}{9004}\sqrt{\frac{15}{14}} & 0 & \frac{28889}{16\sqrt{2}}
\end{pmatrix}
\] (32)

As for \( x^3 \) we get the energies \( E \) by including the first \( N = 1, ..., 5 \) Sturmians also shown in table 2. As is apparent from the table, the ground state values are unstable, i.e., the approximation has failed to converge. This is in sharp contrast to what is known to be the case for the Coulomb and Yukawa potentials (both in their single as in their many-center form) where the convergence is very rapid. This failure can be traced back to the non-convergence of the matrix elements \( W^{(k)}_{nn'} \to \infty \) for \( n, n' \to \infty \), which again is a consequence of the divergent behaviour of the potentials as \( x \to \infty \). Although the Coulomb and Yukawa potentials are singular at the origin, \( r = 0 \), their matrix elements none the less fall of rather rapidly as the quantum numbers increase, due to the quick fall-off of the potentials themselves as \( r \) increases.

Standard perturbation theory would give a value for the ground state energy
in the two cases of

\[
E'_0 = E_0 - \frac{11}{8} \frac{\hbar^2 \alpha^2}{m^3 \omega^4} \quad \text{(cubic potential)} \tag{33}
\]

\[
E'_0 = E_0 + \frac{3}{16} \frac{\hbar^2 \alpha}{m^2 \omega^2} - \frac{23}{4} \frac{\hbar \alpha^2}{m^2 \omega^3} \quad \text{(quartic potential)} \tag{34}
\]

by going to second order in the coupling constant \( \epsilon \) and using standard Rayleigh-Schrödinger perturbation theory, which gives a non-convergent series – for the particular example of \( m = \hbar = \omega = 1, \alpha = .1 \) we get \( E'_0 = 0.3625 \) for the cubic and \( E'_0 = 0.46125 \) for the quartic anharmonic oscillator. Clearly, this is not in good agreement with the result found by using Sturmians, but as will be seen below, this is due to the divergence of the perturbation series. That the Sturmian method is non-perturbative is suggested by the general solution of the secular equation, for the quartic anharmonic potential the ground state energy as a function of \( \alpha \) is found to be (for \( N = 1 \))

\[
E_0 = z^{1/3} + \frac{1}{12} z^{-1/3}
\]

where

\[
z = \frac{2}{2592 \alpha + \sqrt{6718464 \alpha^2 - 6912}}
\]

Such a dependence of \( E \) on \( \alpha \) can only be obtained in perturbation theory by performing at least a partial resummation of the infinite series. That the perturbation series is divergent is mirrored in the behaviour of \( E'_0 \) as a function of the coupling constant \( \alpha \): As \( \alpha \) increases so does the real part of \( E'_0 \). Furthermore, \( E'_0 \) has a small imaginary part which is wildly oscillating but vanishes for \( \alpha > 0.003 \) and hence quickly becomes unimportant. Thus, we must compare our Sturmian energies with non-perturbative results. The divergence of the perturbation series can be improved in a number of ways, as done recently by Bender and Bettencourt, [8], and by Kunihiro, [9]. The latter paper performs a re-summation of the perturbation series by using a renormalisation group (RG) improved technique. From this very rapid expressions for the ground state energy for the quartic anharmonic oscillator is found. Some high-precision numerical results for the quartic anharmonic oscillator have been found by Bacus et al., [10], and we will make a comparison with those findings. Other recent papers on related topics are [11].

We will go back to the original secular equation, (7), and let \( E \) be the energy
of the harmonic oscillator. When \( E = E_n = (n + 1/2)\hbar\omega \) we get \( \beta_n = 1 \) (we will say we are “on shell”) and the secular equation simplifies, since the results then no-longer depend on the normalisation factor \( N_n \propto E^{-3/2} \). Let the number of Sturmians in our basis set be \( N \), then for \( N = 1 \) we get simply

\[
E' = E + \alpha \frac{\langle \psi_n | x^4 | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle} \equiv E + \alpha T_{nn}^{-1} W_{nn}^{(4)} \tag{35}
\]

Let \( N = 2 \) and let the basis set correspond to the quantum numbers \( n, n+1 \), we then find \( E' \) by solving the quadratic equation

\[
0 = (E - E')^2 T_{nn} T_{n+1,n+1} + \alpha(E - E')(T_{nn} W_{n+1,n+1}^{(4)} + T_{n+1,n+1} W_{nn}^{(4)}) + \alpha^2 W_{nn}^{(4)} W_{n+1,n+1}^{(4)} \tag{36}
\]

For \( n = 0, 1, ..., 4 \) we get the results shown in the table 3, where we also show the highly accurate (approx. 90 significant digits) of Bacus et al.. We note that this crude Sturmian approximation is able to get the right order of magnitude for the energy states even of the excited states, but we also notice that the accuracy decreases as \( n \) increases. This is once more due to the non-convergence of the matrix elements of the perturbation potential. Increasing the basis set will not lead to improved accuracy, but can in fact lead to quite the opposite because of this divergence. Hence, the best results are found by the simplest approximation, namely \( N = 1 \). In contrast to the case of asymptotically well-behaved potentials such as the Coulomb and Yukawa ones, hitherto studied in the literature.

4 A Comment on Time Dependent Potentials: The Damped Oscillator

Another important variant of the harmonic oscillator is the damped oscillator. The particular Hamiltonian we’re going to study is the so-called Caldirola-Kanai oscillator, [12],

\[
H = \frac{p^2}{2} e^{-2\gamma t} + \frac{1}{2} \omega x^2 e^{2\gamma t} \tag{37}
\]
where $\gamma$ is some constant, the friction the coefficient and $t$ denotes time. This can be re-expressed in terms of a potential $V'$

$$V' = \frac{1}{2} \omega^2 x^2 e^{2\gamma t'(t)} \equiv \xi(t)V_0(x)$$

(38)

with

$$t'(t) = \frac{1 - e^{-2\gamma t}}{\gamma}$$

(39)

For time dependent potentials $V'$, the secular equation have to be modified. The Schrödinger equation for the full system reads

$$(D + V_0 + V'(t))\psi = i\hbar \frac{\partial}{\partial t}\psi$$

(40)

expanding $\psi = \sum_n c_n(t)\psi_n$ leads to the modified secular equation

$$\sum_n [(1 - \beta_n)N_n\delta_{nn'} + \langle \psi_n' | V'(t) | \psi_n \rangle + E\langle \psi_n' | \psi_n \rangle] c_n = i\hbar \sum_n \xi_n \langle \psi_n' | \psi_n \rangle$$

(41)

Using the relationship between $V'$ and $V_0$ we can rewrite this as

$$\sum_n [(1 - \beta_n(1 + \xi(t)))N_n\delta_{nn'} + E\langle \psi_n' | \psi_n \rangle] c_n = i\hbar \sum_n \xi_n \langle \psi_n' | \psi_n \rangle$$

(42)

For the simplest possible case of only including $N = 1$ Sturmians in the basis set, the solution to this secular equation is of course

$$c_n(t) = c_n(0) \exp \left(-i\hbar \left[(1 - \beta_n)\frac{N_n}{T_{nn}} + E\right] - i(1 - \beta_n)\frac{N_n}{T_{nn}} \int_0^t \xi(t') dt'\right)$$

(43)

It turns out that one can actually compute the integral, since

$$\xi(t) = e^{2 - 2e^{-2\gamma t}}$$

and the integral can be expressed in terms of the exponential integral function leading to

$$c_n(t) = c_n(0) e^{-i\omega_0 t - i\omega(t)}$$

(44)

where

$$\omega_0 = (1 - \beta_n)\frac{N_n}{T_{nn}} + E$$

(45)

$$\omega(t) = (1 - \beta_n)\frac{N_n}{T_{nn}} \frac{e^2}{2\gamma} \left(\text{Ei}(-2) - \text{Ei}(-2e^{-2\gamma t})\right)$$

(46)
Naturally, “on shell” (i.e., for $\beta_n = 1$) we simply get $c_n(t) = c_n(0)e^{-iE_t}$ as one would expect, whereas “off shell” (i.e., for $\beta_n \neq 1$) we get a highly oscillatory behaviour. The explicit results for $N = 1, n = 0$ are $\omega_0 = \frac{1+4E^2}{8E}, \omega(t) = e^{i(1-4E^2)}(Ei(-2) - Ei(-2e^{-2\omega t}))$. One should also notice that this result holds even for $N \neq 1$, one must then interpret the division by $T_{nn}$ as multiplication from the left by the inverse $T_{nn}^{-1}$, whereby $\omega_0, \omega(t)$ become matrices.

The real and imaginary parts of $c_0(t)\psi_0(x)$ have been plotted in figure 2a-b. We notice that the oscillations in the $t$-direction die out either as $x$ increases (because of the decrease of $\psi_0(x)$) or as time goes.

This simple example shows how time-dependent problems simplify in the Sturmian approach because of the simplification of the secular equation. Thus, Sturmians are well suited for problems with time-dependent potentials or for scattering processes. But they are of course subject to the same limitations as in the time-independent case.

It also shows that this particular time-dependent damped oscillator is exactly solvable using the Sturmian approach.

5 A Bath of Harmonic Oscillators

Consider the potential

$$V = \frac{1}{2} \sum_i g_i (x - x_i)^2$$

where $i$ runs over some index set. This represents the potential coming from a family, indexed by $i$, of harmonic oscillators situated at $x_i$ and with coupling constants (characteristic frequencies) $g_i$. We will usually restrict ourselves to $i$ being discrete corresponding to an infinite lattice of oscillators, but for field theoretical purposes it can also be relevant to allow $i$ to run over a continuous index set (in which case the sum must be interpreted as an integral). This example is the harmonic oscillator analogue of the many centre Coulomb potential treated in [4, 5]. Note that we can rewrite $V$ as

$$V = \frac{1}{2} \tilde{g} x^2 - x \sum_i g_i x_i + \frac{1}{2} \sum_i g_i x_i^2$$

$$\equiv \tilde{g} V_0 - xc_1 + c_2$$
where $\bar{g} = \sum_i g_i, c_1 = \sum_i g_i x_i, c_2 = \frac{1}{2} \sum_i g_i x_i^2$, hence we can see this as a perturbation of the original potential $V_0$. Because of this feature of the bath of harmonic oscillators, our computations will simplify somewhat from the many-centre Sturmians introduced for the Coulomb potential in [4, 5], which is very fortunate since those papers use a Fourier transform approach which is not useful for the harmonic oscillator – as mentioned earlier, the Fourier transform, $V’(k)$, of the potential $V$ is a differential operator for the harmonic oscillator (actually, the Hamiltonian is form-invariant under Fourier transforms).

Furthermore, we can complete the squares to write $V$ as another harmonic oscillator plus a constant, in fact

$$V = \frac{1}{2} \bar{g} \left( x - \frac{c_1}{2 \bar{g}} \right)^2 + c_2 - \frac{c_1^2}{4 \bar{g}}$$

Consequently, we can obtain a solution to the many-centre Schrödinger equation by simply making the following substitutions in the solution for the single harmonic oscillator

$$x \rightarrow x + \frac{c_1}{2 \bar{g}}, \quad \beta_n \rightarrow \tilde{\beta}_n, \quad E \rightarrow E - c_2 + \frac{c_1^2}{4 \bar{g}}$$

i.e., the new $\beta_n, \tilde{\beta}_n$ reads

$$\tilde{\beta}_n = \bar{g} \left( \frac{E - c_2 + \frac{c_1^2}{4 \bar{g}}}{n + 1/2} \right)^2$$

Hence the Sturmians read

$$\Psi_n(x; x_i) = \pi^{-1/4}(n!)^{-1/2}2^{-n/2}H_n\left(\beta_1^{1/4}(x + \frac{c_1^2}{4 \bar{g}})\right)e^{-\frac{1}{2}\sqrt{\beta_n(x + \frac{c_1^2}{4 \bar{g}})^2}}$$

These are then a convenient basis for many-centre problems.

For the many-centre Coulomb potential, the Sturmians become related to the one-centre Sturmians by means of phase factors $e^{ikn x_i}$, whereas for the harmonic oscillators the many-centre Sturmians are related to the one-centre ones by means of a translation $x \rightarrow x - \frac{c_1^2}{4 \bar{g}}$ as well as a scaling and a shift in energy.

As a simple example, consider a particle moving in a potential coming from
harmonic oscillators situated at \(x_i = i, i = 1, \ldots, M\) all with equal strengths, \(g_i = 1\). Then \(\bar{g} = M, c_1 = \frac{1}{2} M(M+1), c_2 = \frac{1}{12} M(M+1)(2M+1)\) and

\[
x \to x + \frac{1}{4} (M+1) \quad E \to E - \frac{1}{48} M(5M^2 + 6M + 1)
\]

thus

\[
\tilde{\beta}_n = M \left( \frac{96E - 2M(5M^2 + 6M + 1)}{48(2n + 1)} \right)^2
\]

and the first two Sturmians read explicitly

\[
\Psi_0(x; x_i) = \pi^{-1/4} \exp \left( -M \frac{48E - M(5M^2 + 6M + 1)}{48} \left( x + \frac{1}{4} (M+1) \right)^2 \right) \\
\Psi_1(x; x_i) = \pi^{-1/4} \frac{1}{6} \sqrt{M(48E - M(5M^2 + 6M + 1))} \left( x + \frac{1}{4} (M+1) \right) \times \exp \left( -M \frac{48E - M(5M^2 + 6M + 1)}{144} \left( x + \frac{1}{4} (M+1) \right)^2 \right)
\]

The energy is found from the Schrödinger equation which leads to the “on shell” condition \(\tilde{\beta}_n = 1\). Consequently, the energy of the \(n\)’th state is

\[
E_n = (n + \frac{1}{2}) \bar{g}^{-1/2} - c_2 + \frac{c_1^2}{4\bar{g}}
\]

irrespective of the number of Sturmians used as the secular equation (by construction) is diagonal. In the particularly simple case of \(M\) evenly spaced oscillators all with the same value of the coupling \(g_i = 1\) reads\(^2\)

\[
E_n = (n + \frac{1}{2}) M^{-1/2} - \frac{1}{12} M(M+1)(2M+1) + \frac{1}{16} M(M+1)^2
\]

which is then the energy of a (non relativistic) particle moving in a one-dimensional lattice of oscillators – a highly simplified model of, say, a particle in a solid. For a many-dimensional lattice we would simply use products of unidimensional Sturmians.

\(^2\)Note, for \(M = 1\), \(E \neq n + 1/2\), because the potential in this instance is \(V = \frac{1}{2}(x-1)^2\) and not \(V = V_0\). Had we instead used \(x_i = i - 1\), we would get \(V(M = 1) = V_0, E(M = 1) = n + 1/2\). In that case, by the way, \(c_1 = \frac{1}{2} M(M-1), c_2 = \frac{1}{12} M(M-1)(2M-1)\).
6 A Comment on Coupled Oscillators

Consider now a potential of the form

\[
V = \frac{1}{2} \sum_i g_i (x - x_i)^2 + \frac{1}{2} \sum_{i \neq j} \lambda_{ij} (x - x_i)^2 (x - x_j)^2
\]  

(57)

which introduces a coupling between the oscillators at the various positions. In a manner similar to the manipulations of the bath of oscillators, this can be transformed into a single anharmonic oscillator potential

\[
V = \frac{1}{2} \bar{g} x^2 - c_1 x + c_2 - c_3 x^3 + c_4 x^4
\]  

(58)

where

\[
\bar{g} = \sum_i g_i \quad (59)
\]

\[
c_1 = \sum_i 2(g_i - \sum_{j \neq i} \lambda_{ij} (x_j^2 + x_j x_i)) x_i \quad (60)
\]

\[
c_2 = \frac{1}{2} \sum_i (g_i + \sum_{j \neq i} x_j^2) x_i^2 \quad (61)
\]

\[
c_3 = \sum_{i \neq j} \lambda_{ij} (x_i + x_j) \quad (62)
\]

\[
c_4 = \frac{1}{2} \sum_{i \neq j} \lambda_{ij} \quad (63)
\]

Suppose \( \chi \) is a solution to the corresponding Schrödinger equation. We can then expand \( \chi \) either on the ordinary Sturmians, \( \psi_n \), or the Sturmians for a bath of oscillators, \( \Psi_n \). If we choose the latter option, we have to complete the squares to obtain the centre of the new oscillator, but this would mean that the anharmonic terms too would have to be shifted and this would again introduce lower powers of the new, shifted position. Hence the secular equation would end up having the same structure and thus the same level of complication. Consequently, nothing is lost by expanding on the single oscillator Sturmians \( \psi_n, \chi = \sum_n \alpha_n \psi_n \). The secular equation then becomes

\[
0 = \sum_{n'} \left[ (\beta_n + \bar{g}) N_n \delta_{nn'} - c_1 W_{nn'}^{(1)} + c_2 T_{nn'} - c_3 W_{nn'}^{(3)} - c_4 W_{nn'}^{(4)} \right] \alpha_{n'} \quad (64)
\]
where

\[ W^{(k)}_{mn'} := \int \psi_n^* x^k \psi_{m'} dx \]  

(65)

is the matrix elements of the \( k \)'th power of \( x \), \( W^{(0)}_{nn'} = T_{nn'} \). The only one of these we do not already know is for \( k = 1 \) in which instance a straightforward computation yields

\[
W^{(1)} = E^{-1} \begin{pmatrix}
0 & \frac{3}{8} & 0 & \frac{-21}{128} \sqrt{3} & 0 \\
\frac{3}{8} & 0 & \frac{75}{128} \sqrt{3} & 0 & \frac{-61}{64 \sqrt{2}} \\
0 & \frac{75}{128} \sqrt{3} & 0 & \frac{1925}{128} \sqrt{3} & 0 \\
\frac{-21}{128} \sqrt{3} & 0 & \frac{1925}{128} \sqrt{3} & 0 & \frac{508599}{131072} \\
0 & \frac{-61}{64 \sqrt{2}} & 0 & \frac{508599}{131072} & 0
\end{pmatrix}
\]  

(66)

for the first five Sturmians. Consequently, for \( N = 1 \) we get (since \( W^{(2k+1)} \) is diagonal)

\[(\beta_n + \bar{g}) N_n + c_2 T_{nn} - c_4 W^{(4)}_{nn} = 0 \]  

(67)

which is a cubic equation for \( E \), e.g. for \( n = 0 \)

\[
\bar{g} - 3c_4 E + 4E^2 + 16c_2 E^3 = 0
\]

which for the extremely simple case of \( \bar{g} = c_2 = c_4 = 1 \) has the three solutions \( E = -0.669498, 0.209749 \pm i0.222168 \), i.e., one negative energy state (hence a bound state) and two complex conjugate oscillatory states.

For \( N = 2 \) and \( \bar{g} = c_i = 1^3 \) leads to the following solutions \( E = -9.91107, -1.51155 \) and \( E = 0.129506 \pm i0.435961, 0.537995 \pm i1.32394 \), which then corresponds to two bound states and two pairs of oscillatory states, the latter of which essentially oscillates around the ground state of the single harmonic oscillator.

7 The Gaussian-Damped Anharmonic Oscillator

The previous computations seem to suggest that the Sturmian method is best suited for potentials which are well behaved at infinity such as the Coulomb

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3Which, by the way, is only possible for two coupled oscillators if \( x_1 = \frac{1}{4}(1 + \sqrt{1 + 8\sqrt{14}}), x_2 = \frac{1}{2} - x_1, g_1 = \frac{1}{4} \pm \frac{23175}{170088} \sqrt{1 + 8\sqrt{14}}, g_2 = 1 - g_1.\)
potential, but very slow converging for potential diverging as \( x \to \infty \) such as the anharmonic oscillator. To test this hypothesis, we will now briefly consider a toy model, the anharmonic oscillator damped by a Gaussian \( V' = ax^k e^{-x^2} \) where \( k = 3, 4 \).\(^4\) Including only the first five Sturmians we get the following matrix elements, \( \tilde{V}^{(k)}_{nm'} \) of \( V' \), \( k = 3, 4 \):

\[
\begin{pmatrix}
0 & \frac{27}{2(3+4E)^{7/2}} & 0 \\
-\sqrt{\frac{3}{2}} \frac{343(3+2E)}{2(7+8E)^{7/2}} & 0 & -\frac{225(15-22E)}{4\sqrt{\frac{1}{8} + \frac{5}{2} (15+8E)^3}} \\
0 & \frac{81(243-324E-52E^2)}{4\sqrt{2+\frac{5}{2}E(9+4E)^4}} & 0 \\
-\sqrt{\frac{3}{2}} \frac{343(3+2E)}{2(7+8E)^{7/2}} & 0 & \frac{225(525-940E+316E^2)\sqrt{21}}{4\sqrt{1+\frac{5}{2}E(35+12E)^4}} \\
0 & \frac{81(243-324E-52E^2)}{4\sqrt{2+\frac{5}{2}E(9+4E)^4}} & 0 \\
-\frac{250017(107163-207522E+94356E^2-13816E^3)}{8(63+16E)^{11/2}} & 0 & 0 \\
\end{pmatrix}
\]

\[ (68) \]

\[
\tilde{V}^{(4)} = \begin{pmatrix}
\frac{3}{4(1+2E)^{7/2}} & 0 & \frac{75(5-4E)}{8\sqrt{\frac{1}{8} + \frac{5}{2} (5+6E)^3}} \\
0 & \frac{5}{2(1+2E)^{7/2}} & 0 \\
\frac{243(243-100E^2)}{16\sqrt{\frac{5}{2} + \frac{5}{2} (9+10E)^4}} & -\frac{19845(21-4E)}{4\sqrt{\frac{1}{8} + \frac{5}{2}E(21+10E)^4}} & \frac{75(258-80E+104E^2)}{8\sqrt{\frac{1}{8} + \frac{5}{2}E(5+4E)^4}} \\
\end{pmatrix}
\]

\[ (69) \]

\(^4\)One could also consider simply the exponentially damped oscillator \( V' = x^k e^{-|x|} \), but due to the presence of the absolute value the matrix elements become too complicated.
which leads to the ground state energies shown in table 4 below. We notice the improved convergence properties supporting our claim that it was the non-convergence of the matrix elements of the undamped anharmonic oscillator that was the cause for the non-convergence of the ground state energies in the Sturmian method.

8 Conclusion

We have seen that the powerful technique of Sturmian functions developed for Coulomb-like potentials can be extended to harmonic and anharmonic oscillators, where it furthermore can be seen that the technique is highly non-perturbative, but the divergence of the potential (as \( x \rightarrow \pm \infty \)) leads to a non-convergence of the Sturmian approximation, in contrast to the Coulomb case, where we have very rapid convergence. It turned out, however, that already with \( N = 1, 2 \) Sturmians the correct order of magnitude for the energies of even the excited states could be obtained. Thus indicating that the problem with convergence is perhaps not so serious after all, if one merely wants to find the order of magnitude. For higher precision, one should probably utilise a hybrid method, using the first few Sturmians to get the correct order of magnitude and then some variational approach, say, to get the required precision.

We also saw how to treat time-dependent problems, where once again the Sturmian properties lead to some important simplifications. Finally, we considered a bath of coupled or uncoupled oscillators which could be transformed into a single anharmonic oscillator problem. This is contrary to what one does for the Coulomb potential, where Fourier transform techniques are used instead. Furthermore, when using a modified (or regularised) potential, convergent at infinity but with the same behaviour for \( x \) not too large, we did
get rapid convergence, especially for the $x^3$ case, whereas the $x^4$ case had
slightly slower convergence.

All of this seems to suggest that the Sturmian techniques have a very wide
range of applicability covering basically all important potentials known in
atomic physics or quantum chemistry, but one should be very careful when
using potentials which are not well behaved at infinity. Given the generality
of the approach, as outlined in the introduction, this procedure should
also be extendible to problems in quantum field theory using a functional
Schrödinger picture and to problems in quantum kinetic theory in phase
space using Wigner functions for instance.

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A Certain Results Concerning Hermite Polynomials

In this appendix we prove a few results concerning Hermite polynomials. The
generating function is known to be

\[ e^{-s^2 + sx} = \sum_{n=0}^{\infty} \frac{s^n}{n!} H_n(x) \]  

(70)

from this it is straightforward to deduce the standard orthonormality relation
for the Hermite polynomials and the harmonic oscillator wave functions. We
will also use it to derive some other useful results.
First we need the Fourier transform of a harmonic oscillator Sturmian. Thus
we want to compute the following integral

\[ \int_{-\infty}^{\infty} e^{ikx} H_n(\alpha x) e^{-\frac{1}{2}\beta x^2} d\alpha \]

The corresponding integral with the generating function is merely a Gaussian
integral and can be readily computed

\[ \int e^{-s^2 + \alpha sx - \frac{1}{2}\beta x^2 + ikx} d\alpha = e^{-s^2} \sqrt{\frac{2\pi}{\beta}} e^{\frac{1}{2}(\alpha + ik)^2} \]  

(71)
from which we get, by Taylor expansion, the desired result:

\[
\int H_n(\alpha x) e^{-\frac{1}{2} k^2 x^2 + ik x} dx = \sqrt{\frac{2\pi}{\beta}} (1 + \frac{\alpha^2}{2\beta})^{\frac{n}{2}} H_n(i k \frac{\alpha}{\beta} (1 + \frac{\alpha^2}{2\beta}))^{-\frac{1}{2}} e^{\frac{1}{2} \frac{1}{\beta} - ik^2}
\]

(73)

Actually, this formula is a little more general than we need. For harmonic oscillator Sturmians it turns out that \( \alpha = \beta = (\beta_m)^{1/4} \) which leads to a slight simplification, resulting in the formula given in the text.

Another expression we need is the matrix element of \( x^n \) for \( \gamma \) some positive integer \( \geq 2 \), i.e., we need to compute

\[
I_{nm}(\alpha, \beta, \gamma, \delta) := \int H_n(\alpha x) H_m(\beta x) x^\gamma e^{-\frac{1}{2} k^2 x^2} dx
\]

(74)

Again, in terms of the generating function, the integral we need to compute is quite simply

\[
\int e^{-2x^2 + 2(\alpha + \beta)x - \frac{1}{2} k^2 x^2} x^\gamma dx = e^{-2x^2 + 2\gamma/2 k^2 - 1 - \gamma/2} \Gamma(1 + \frac{\gamma}{2}) \times
\]

\[
\left(2(\alpha + \beta)s(1 - (-1)^\gamma) \right) e \left( 2(\alpha + \beta) s^2 \right) +
\]

\[
(1 + (-1)^\gamma) \sqrt{\frac{\delta \pi}{2}} e^{2(\alpha + \beta) s^2} L_{\frac{1}{2}}^{-\frac{1}{2}}(2(\alpha + \beta) s^2)
\]

\[
\equiv I(\alpha, \beta, \gamma, \delta)
\]

(75)

(76)

which is valid even for non-integer \( \gamma \). Here \(_1 F_1\) is a hypergeometric function and \( L_a^b\) is an associated Laguerre polynomial. The first few of these are

\[
L_1^{-1/2}(x) = \frac{1}{2} - x
\]

\[
L_2^{-1/2}(x) = \frac{1}{8} (3 - 12x + 4x^2)
\]

\[
L_3^{-1/2}(x) = \frac{1}{48} (15 - 90x + 60x^2 - 8x^3)
\]

\[
_1 F_1\left(\frac{3}{2}, \frac{3}{2}; x\right) = e^x
\]

23
\[ _1F_1 \left( \frac{5}{2}; \frac{3}{2}; x \right) = \frac{1}{3} e^x (3 + 2x) \]
\[ _1F_1 \left( \frac{7}{2}; \frac{3}{2}; x \right) = \frac{1}{15} e^x (15 + 20x + 4x^2) \]

For the two cases of interest to us, \( \gamma \) an even or odd positive integer, we get a simpler relation since one of the two terms on the right hand side will vanish.

For \( \gamma = 2k \) we arrive at
\[
I(\alpha, \beta, 2k, \delta) = 2^{k+1} e^{-2x^2} \delta^{-1-k} k! \sqrt{\frac{1}{2\pi \delta}} e^{2(\alpha+\beta)^2 \delta} I_k \left( -2 \frac{(\alpha + \beta)^2 \delta^2}{\delta} \right)
\]
whereas for \( \gamma = 2k + 1 \) find
\[
I(\alpha, \beta, 2k+1, \delta) = 2^{k+5/2} e^{-2x^2} \delta^{-k-3/2} \Gamma(k+\frac{3}{2}) s(\alpha+\beta) I_1(k+\frac{3}{2}; \frac{3}{2}; \frac{(\alpha + \beta)^2 \delta^2}{\delta})
\]

Taylor expanding in \( s \), we get
\[
I(\alpha, \beta, \gamma, \delta) \equiv \sum_{n=0}^{\infty} I_n(\alpha, \beta, \gamma, \delta) s^n n! = \sum_{n,m=0}^{\infty} \frac{s^{n+m}}{n! m!} I_{nm}(\alpha, \beta, \gamma, \delta) \quad (77)
\]

From this we can obtain relationships between the matrix elements \( W_{nm}^{(k)} \) for different \( k \)'s, since \( I_{nm} \propto W_{nm}^{(k)} \) for \( \alpha = \beta_n^{1/4}, \beta = \beta_m^{1/4} \). For instance
\[
I_{00} = I_0 \\
I_{01} + I_{10} = I_1 \\
\frac{1}{2} I_{02} + \frac{1}{2} I_{11} = \frac{1}{2} I_2 \\
\frac{1}{6} (I_{03} + I_{30}) + \frac{1}{2} (I_{21} + I_{12}) = \frac{1}{6} I_3
\]
such rules (essentially following from the recursion relation for the Hermite polynomials) can be used to simplify the computation of matrix elements.

One should also note that, since the above is valid even for \( \gamma \) not a positive integer, we can use it to obtain the matrix elements of the Coulomb potential between harmonic oscillator Sturmians.
References


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Table 1: Normalisation constants for harmonic oscillator Sturmians.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$N_n$</th>
<th>$n$</th>
<th>$N_n$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$\frac{1}{\sqrt{2}} E^{-3/2}$</td>
<td>5</td>
<td>$\frac{121}{8} \sqrt{\frac{11}{2}} E^{-3/2}$</td>
</tr>
<tr>
<td>1</td>
<td>$\frac{9}{8} \sqrt{\frac{3}{2}} E^{-3/2}$</td>
<td>6</td>
<td>$\frac{169}{8} \sqrt{\frac{13}{2}} E^{-3/2}$</td>
</tr>
<tr>
<td>2</td>
<td>$\frac{25}{8} \sqrt{\frac{5}{2}} E^{-3/2}$</td>
<td>7</td>
<td>$\frac{225}{8} \sqrt{\frac{15}{2}} E^{-3/2}$</td>
</tr>
<tr>
<td>3</td>
<td>$\frac{49}{8} \sqrt{\frac{7}{2}} E^{-3/2}$</td>
<td>8</td>
<td>$\frac{289}{8} \sqrt{\frac{17}{2}} E^{-3/2}$</td>
</tr>
<tr>
<td>4</td>
<td>$\frac{243}{8} \sqrt{\frac{9}{2}} E^{-3/2}$</td>
<td>9</td>
<td>$\frac{361}{8} \sqrt{\frac{19}{2}} E^{-3/2}$</td>
</tr>
</tbody>
</table>

Table 2: The energies for the cubic and quartic anharmonic oscillator $V' = \alpha x^3, \alpha x^4$ with $\alpha = 0.1$ found by using only the first $N$ Sturmians. Only the ground state energies are shown.

\begin{tabular}{|c|c|c|}
\hline
$N$ & $E(x^3)$ & $E(x^4)$ \\
\hline
1 & 0.500000 & 0.562709 \\
2 & 0.014628 & 0.562709 \\
3 & 0.112767 & 0.562709 \\
4 & 0.351135 & 0.562544 \\
5 & 0.102981 & 0.562516 \\
10 & 1.27012 & 0.533858 \\
\hline
\end{tabular}
Table 3: A comparison between the perturbed energy states for the quartic anharmonic oscillator with $\alpha = .1$ found by using two Sturmians and the high-precision results of Bacus et al., the second order perturbative result for this case $(m = \frac{1}{2}, \omega = 2)$ is $E_0 = 0.4900$ for the ground state.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$E$ (Sturmian) $N = 1$</th>
<th>$E$ (Bacus) $N = 2$</th>
<th>difference $N = 1$</th>
<th>$N = 2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.07500</td>
<td>1.07500</td>
<td>-0.00971</td>
<td>-0.00971</td>
</tr>
<tr>
<td>1</td>
<td>3.37500</td>
<td>3.30687</td>
<td>-0.06813</td>
<td>-0.06813</td>
</tr>
<tr>
<td>2</td>
<td>5.97500</td>
<td>5.74795</td>
<td>-0.22705</td>
<td>-0.22705</td>
</tr>
<tr>
<td>3</td>
<td>8.87500</td>
<td>8.35268</td>
<td>-0.52232</td>
<td>1.35116</td>
</tr>
<tr>
<td>4</td>
<td>12.07500</td>
<td>11.09860</td>
<td>-0.97640</td>
<td>1.79767</td>
</tr>
</tbody>
</table>

Table 4: The ground state energies for $V' = x^k e^{-x^2}, k = 3, 4$ computed using $N$ Sturmians.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$E(x^3)$</th>
<th>$E(x^4)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.500000</td>
<td>0.622877</td>
</tr>
<tr>
<td>2</td>
<td>0.495852</td>
<td>0.622877</td>
</tr>
<tr>
<td>3</td>
<td>0.491822</td>
<td>0.622878</td>
</tr>
<tr>
<td>4</td>
<td>0.491282</td>
<td>0.622877</td>
</tr>
<tr>
<td>5</td>
<td>0.491282</td>
<td>0.622878</td>
</tr>
</tbody>
</table>

Figure 1: A plot of the first ten harmonic oscillator Sturmians showing how they are scaled to all have essentially the same range.
Figure 2: The real (a) and imaginary (b) parts of the first time dependent Sturmian for the damped (Caldirola-Kanai) oscillator, \( c_\alpha(t)\psi_0(x) \), in the range \( t \in [0, 10], x \in [0, 5] \) and with \( E = \gamma = 1 \).