Sturmian basis functions for the harmonic oscillator

Frank Antonsen*
Niels Bohr Institute, Blegdamsvej 17, DK-2100 Copenhagen, Denmark
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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 nonperturbative 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. [S1050-2947(99)10107-0]

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I. INTRODUCTION

A typical situation in quantum theory is to be faced with a physical potential V for which one has to solve the corresponding wave equation to find 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 $V_0(x_1,\ldots,x_N)$. The eigenvalue equation for the Hamiltonian (wave equation) is then an equation of the general form

$$(D+V_0-E)\psi=0, \tag{1}$$

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

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

(2) The Schrödinger equation $D=(1/2m)\nabla^2$ where ∇^2 is the Laplace operator in d dimensions.

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

For $N>1$ we simply have $D=\Sigma_{i=1}^{N}D_i$ where D_i is the appropriate operator for the ith particle. Thus all relativistic as well as nonrelativistic quantum mechanics fall into this category (even in curved space-times). One then typically proceeds by trying to find a complete set of eigenstates corresponding to the different values of E; when D is Hermitian these form an orthonormal set.[1] The problem is, however, that for many cases continuous as well as discrete eigenvalues have to be taken into account in order to obtain a basis for the full Hilbert space. This is, for instance, the case in the Coulomb potential case already in nonrelativistic quantum mechanics, where continuum eigenstates are needed to obtain completeness. Consequently, alternatives will have to be found. Shull and Löwdin [1] introduced another approach for the Coulomb potential. Their methods were generalized by Rotenberg, who also coined the word ''Sturmians'' for the new basis set [2]. It has recently been realized that this approach can be even further generalized to handle, e.g., many center 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.

The structure of the paper is as follows. First we outline the general Sturmian machinery and derive the most important properties of these kinds of functions, then we find the explicit formula for the Sturmians corresponding to the harmonic-oscillator potential. Next we consider the anharmonic oscillator, and show that our approach amounts to a nonperturbative calculation which, however, is merely an asymptotic series and not a converging one. This is due to the divergence of the matrix elements of the potential. Some comments are made on generalizations to the many-particle case and to time-dependent potentials (the Caldirola-Kanai oscillator), and finally we show that the nonconvergence can be remedied by considering appropriately ''regularized'' potentials involving a Gaussian regulator.

*Electronic address: Antonsen@alf.nbi.dk

[1]Actually, for the Klein-Gordon case, hermiticity is more subtle and depends on a precise definition of the inner product, but for the Schrödinger equation (and the Dirac equation), which is the only one we will be using in this paper, such subtleties are absent and D is indeed Hermitian. Moreover, by reformulating everything in terms of an appropriate inner product instead of the usual L^2 one used here, one can verify that Klein-Gordon Sturmians have properties like those derived in this paper.

II. BASIC PROPERTIES OF STURMIANS

Instead of finding a set of eigenfunctions all corresponding to the same ''coupling 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

$$(D+\beta_{\mathbf{n}}V_0-E)\psi_{\mathbf{n}}=0, \tag{2}$$

where $\beta_{\mathbf{n}}$ is some constant depending on the set $\mathbf{n}$ of quantum numbers. The solution of this equation gives E as a function of $\beta_{\mathbf{n}}$ which can then be inverted to find $\beta_{\mathbf{n}}$ as a function of E, assuming we can solve Eq. (2), of course. We will refer to $\beta_{\mathbf{n}}$ as the *effective coupling constant*—for $V_0=-Z/r$ it corresponds to scaling the nuclear charge, and for $V_0=m\omega^2x^2$ it corresponds to scaling the mass and/or the frequency.

The assumed hermiticity of D then implies

$$(\beta_{\mathbf{n}}-\beta_{\mathbf{n}'})\int \psi^*_{\mathbf{n}'}V_0\psi_{\mathbf{n}}dx=0, \tag{3}$$

i.e., the Sturmian functions satisfy the potential weighted orthogonality relation

$$\int \psi^*_{\mathbf{n}}V_0\psi_{\mathbf{n}'}dx=N_{\mathbf{n}}\delta_{\mathbf{n}\mathbf{n}'}. \tag{4}$$

Strictly speaking, Eq. (3) only implies $\int\psi^*_{\mathbf{n}'}V_0\psi_{\mathbf{n}}dx=0$ for $\beta_{\mathbf{n}}\neq\beta_{\mathbf{n}'}$. For sufficiently nice potentials, i.e., potentials without any violent oscillations, such that the energy E depends monotonically on the quantum numbers $\mathbf{n}$, the orthonormality condition (4) follows. An example of a potential which we do not expect to be able to handle with this approach is $V_0(x)=\sin x/x$, but potentials x^{-1}, $x^{-1}e^{-kx}$, and x^2 can be treated this way. It will also be shown later that the many-center analogs of these potentials are also within reach. Another subtlety concerns ''major'' and ''minor'' quantum numbers in the terminology of Aquilanti and Avery [5]. The coefficient $\beta_{\mathbf{n}}$ need not depend on all quantum numbers; those on which it does depend are referred to as ''major'' quantum numbers, and the remaining ones are then ''minor'' quantum numbers. For the Coulomb potential, for instance, $\beta_{\mathbf{n}}$ only depends on n and not on the angular momentum quantum numbers l and m. The orthogonality with respect to the minor quantum numbers then follow from the orthonormality of the spherical harmonics Y_{lm} and the separation of variables, $\psi_{\mathbf{n}}(r,\Omega)=\chi_{nl}(r)Y_{lm}(\Omega)$. For one-dimensional systems, no such subtlety can occur. Although we will make some comments on many-particle and many-center Sturmians, which correspond to higher dimensions, we will not encounter this subtlety in this paper.

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. If E is taken to be the actual physical energy the Sturmians will, furthermore, have the right asymptotic behavior. 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 $V_0\sim x^2$).[2] The eigenvalue equation for the Hamiltonian, $H=D+V_0+V'$, for this new system is then

$$(D+V_0+V'-E')\psi=0. \tag{5}$$

Suppose we can expand ψ on the Sturmians for V as $\psi=\sum_{\mathbf{n}}c_{\mathbf{n}}\psi_{\mathbf{n}}$,[3] we then obtain

$$(D+V_0+V'-E')\sum_{\mathbf{n}}c_{\mathbf{n}}\psi_{\mathbf{n}}$$

$$=\sum_{\mathbf{n}}c_{\mathbf{n}}[(1-\beta_{\mathbf{n}})V_0+V'+E-E']\psi_{\mathbf{n}} \tag{6}$$

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

$$\sum_{\mathbf{n}}[(1-\beta_{\mathbf{n}})N_{\mathbf{n}}\delta_{\mathbf{n}\mathbf{n}'}+\langle\psi_{\mathbf{n}'}|V'|\psi_{\mathbf{n}}\rangle$$

$$+(E-E')\langle\psi_{\mathbf{n}'}|\psi_{\mathbf{n}}\rangle]c_{\mathbf{n}}=0, \tag{7}$$

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. We can rewrite this equation as

$$E'=E+\frac{[(1-\beta_{\mathbf{n}'})N_{\mathbf{n}'}+\langle\psi_{\mathbf{n}'}|V'|\psi_{\mathbf{n}'}\rangle]c_{\mathbf{n}'}+\sum_{\mathbf{n}\neq\mathbf{n}'}\langle\psi_{\mathbf{n}'}|V'|\psi_{\mathbf{n}}\rangle c_{\mathbf{n}}}{\langle\psi_{\mathbf{n}'}|\psi_{\mathbf{n}'}\rangle+\sum_{\mathbf{n}\neq\mathbf{n}'}\langle\psi_{\mathbf{n}'}|\psi_{\mathbf{n}}\rangle c_{\mathbf{n}}} \tag{8}$$

[2]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, in order to be able to make a comparison with perturbation theory.

[3]For one-dimensional systems, it follows from standard Sturm-Liouville theory that the Sturmians do form a basis. Furthermore, for the case of radial potentials in higher dimensions this is also known to be the case.

$$\equiv E+\frac{[(1-\beta_{\mathbf{n}'})N_{\mathbf{n}'}+W_{\mathbf{n}'\mathbf{n}'}]c_{\mathbf{n}'}+\sum_{\mathbf{n}\neq\mathbf{n}'}W_{\mathbf{n}'\mathbf{n}}c_{\mathbf{n}}}{T_{\mathbf{n}'\mathbf{n}'}c_{\mathbf{n}'}+\sum_{\mathbf{n}\neq\mathbf{n}'}T_{\mathbf{n}'\mathbf{n}}c_{\mathbf{n}}}, \tag{9}$$

where we have defined the overlap matrices

$$T_{\mathbf{n}'\mathbf{n}}:=\langle\psi_{\mathbf{n}'}|\psi_{\mathbf{n}}\rangle, \tag{10}$$

$$W_{\mathbf{n}'\mathbf{n}}:=\langle\psi_{\mathbf{n}'}|V'|\psi_{\mathbf{n}}\rangle. \tag{11}$$

The secular equation often implies that one can find E' with very great accuracy from an extremely small basis set, even with just one basis function, $\psi_{\mathbf{n}}$, in which case we have simply

$$E'=\frac{(1-\beta_{\mathbf{n}})N_{\mathbf{n}}-\langle\psi_{\mathbf{n}}|(V'-E)|\psi_{\mathbf{n}}\rangle}{\langle\psi_{\mathbf{n}}|\psi_{\mathbf{n}}\rangle},$$

giving an explicit formula for E', which, when V' is sufficiently close to V_0 and the potentials are sufficiently well behaved, is a surprisingly good fit [4,7]. The reason for this success is to be found in the very nature of Sturmian basis sets. 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 optimized 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

$$E_0\leqslant\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle};$$

with $\psi=\psi_{\mathbf{n}}$, a Sturmian, we obtain

$$E_0\leqslant E+(1+\beta_{\mathbf{n}})\frac{\langle\psi_{\mathbf{n}}|V_0|\psi_{\mathbf{n}}\rangle}{\langle\psi_{\mathbf{n}}|\psi_{\mathbf{n}}\rangle}+\frac{\langle\psi_{\mathbf{n}}|V'|\psi_{\mathbf{n}}\rangle}{\langle\psi_{\mathbf{n}}|\psi_{\mathbf{n}}\rangle}, \tag{12}$$

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 obtain

$$E_0\leqslant E+\beta_{\mathbf{n}}\frac{\langle\psi_{\mathbf{n}}|V_0|\psi_{\mathbf{n}}\rangle}{\langle\psi_{\mathbf{n}}|\psi_{\mathbf{n}}\rangle}+\frac{\langle\psi_{\mathbf{n}}|V'|\psi_{\mathbf{n}}\rangle}{\langle\psi_{\mathbf{n}}|\psi_{\mathbf{n}}\rangle}, \tag{13}$$

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

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

Since the above consideration only used the fact that D was Hermitian, the results hold for all the above-mentioned cases provided we can find effective couplings $\beta_{\mathbf{n}}$ such that E can be held fixed. It is known that such $\beta_{\mathbf{n}}$ exist for the Coulomb and Yukawa potentials both in relativistic (the Dirac equation) and nonrelativistic quantum mechanics and also for their many-center analogs. 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. We write the original potential as $V_0(x)=\alpha v(x)$, where α 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, choices for α and for the set of quantum numbers $\mathbf{n}$ uniquely specify the energy E, and thus we can invert the relation to find α as a function of E and $\mathbf{n}$. If there is degeneracy, the equation $\alpha=\alpha(E,\mathbf{n})$ has more than one solution in the physical range, but this merely means that more than one set of quantum numbers exists giving the same energy; for each such choice of quantum numbers we obtain a new solution $\beta_{\mathbf{n}}=\alpha(E,\mathbf{n})$.

Another interesting relationship is the momentum space orthonormality relation. Let $\phi_{\mathbf{n}}(k)$ be the Fourier transform of $\psi_{\mathbf{n}}(x)$; this then satisfies

$$(D^t-E)\phi_{\mathbf{n}}=-\beta_{\mathbf{n}}V_0^t*\phi_{\mathbf{n}}, \tag{14}$$

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

$$V_0^t*\phi_{\mathbf{n}}=\int V_0^t(k-k')\phi_{\mathbf{n}}(k')dk'. \tag{15}$$

We multiply by $\phi_{\mathbf{n}'}^*$ from the left, and perform the k integral to arrive at

$$\int\phi_{\mathbf{n}'}^*(D^t-E)\phi_{\mathbf{n}}dk=-\beta_{\mathbf{n}}\int\phi_{\mathbf{n}'}^*(V_0^t*\phi_{\mathbf{n}})dk. \tag{16}$$

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

$$\int\phi_{\mathbf{n}'}^*(D^t-E)\phi_{\mathbf{n}}dk=-\beta_{\mathbf{n}}N_{\mathbf{n}}\delta_{\mathbf{n}\mathbf{n}'}. \tag{17}$$

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

$$\int \phi^*_{\mathbf{n}'}(\gamma^0\gamma^\mu k_\mu - E - \gamma^0 m)\phi_n dk = -\beta_{\mathbf{n}} N_{\mathbf{n}} \delta_{\mathbf{n}\mathbf{n}'},$$

$$\int \phi^*_{\mathbf{n}'}(k^2 - 2mE)\phi_{\mathbf{n}} dk = -2m\beta_{\mathbf{n}} N_{\mathbf{n}} \delta_{\mathbf{n}\mathbf{n}'},$$

$$\int \phi^*_{\mathbf{n}'}(k^2 - m^2 - E)\phi_{\mathbf{n}} dk = -\beta_{\mathbf{n}} N_{\mathbf{n}} \delta_{\mathbf{n}\mathbf{n}'}$$

for the Dirac, Schrödinger, and Klein-Gordon equations, respectively. In the nonrelativistic 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 found the existence of SO(4) symmetry. This can be generalized to arbitrary dimensions by means of hyperspherical harmonics [3,4].

The momentum-space relations have other important implications. The eigenvalue equation of the Hamiltonian in momentum space is

$$(D^t - E)\phi_{\mathbf{n}}(k) = -\beta_{\mathbf{n}} V_0^t * \phi_{\mathbf{n}}. \tag{18}$$

We define, for simplicity, $\tilde{\phi}_{\mathbf{n}} = (D^t - E)\phi_{\mathbf{n}}$; then we can write the momentum-space orthonormality relation as $\int \phi^*_{\mathbf{n}} \tilde{\phi}_{\mathbf{n}'} dk = -\beta_{\mathbf{n}} N_{\mathbf{n}} \delta_{\mathbf{n}\mathbf{n}'}$ and the eigenvalue equation for the Hamiltonian as

$$\tilde{\phi}_{\mathbf{n}}(k) = -\beta_{\mathbf{n}}(V_0^t * \phi_{\mathbf{n}})(k) \tag{19}$$

$$= -\beta_{\mathbf{n}} \int V_0^t(k - k')\phi_{\mathbf{n}}(k') dk'. \tag{20}$$

Now, we make the following ansatz:

$$V_0^t(k - k') = \sum_{\mathbf{n}} c_{\mathbf{n}} \tilde{\phi}_{\mathbf{n}}(k) \tilde{\phi}^*_{\mathbf{n}}(k'). \tag{21}$$

Inserting this into Eq. (20) we then obtain

$$c_{\mathbf{n}} = \frac{N_{\mathbf{n}}}{\beta_{\mathbf{n}}^2}, \tag{22}$$

i.e.,

$$V_0^t(k - k') = \sum_{\mathbf{n}} \frac{N_{\mathbf{n}}}{\beta_{\mathbf{n}}^2} \tilde{\phi}_{\mathbf{n}}(k) \tilde{\phi}^*_{\mathbf{n}}(k') \tag{23}$$

$$:= \sum_{\mathbf{n}} \frac{N_{\mathbf{n}}}{\beta_{\mathbf{n}}^2} D^t(k)(D^t(k'))^* \phi_{\mathbf{n}}(k) \phi^*_{\mathbf{n}}(k'). \tag{24}$$

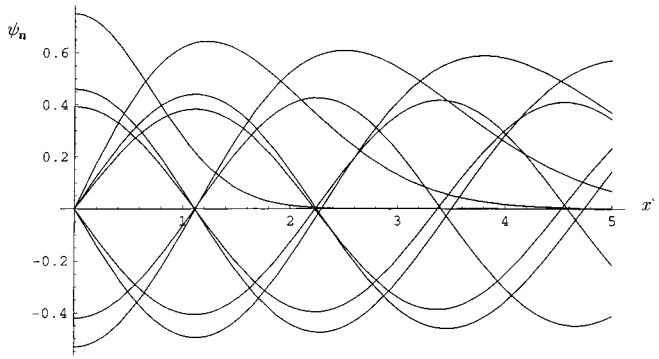

FIG. 1. Plot of the first ten harmonic-oscillator Sturmians showing how they are scaled to all have essentially the same range.

When V_0^t is some function of k and k', this is a useful summation formula for the momentum-space Sturmians. When V_0^t 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 emphasized 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 normalization, the ''effective charge'' $\beta_{\mathbf{n}}$, 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.

III. 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

$$\left(-\frac{1}{2m}\frac{d^2}{dx^2} + \frac{1}{2}\beta_{\mathbf{n}} x^2 - E \right) \psi_{\mathbf{n}} = 0, \tag{25}$$

which is the harmonic oscillator Schrödinger equation with $m\omega^2$ replaced by $\beta_{\mathbf{n}}$. We will henceforth use mass weighted coordinates and set $m=1$; if the mass needs to be reinstated

TABLE I. Normalization constants for harmonic-oscillator Sturmians.

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

one simply replaces x by $\sqrt{m}x$. In this case ω in the original harmonic-oscillator Hamiltonian has been replaced by $\beta_{\mathbf{n}}^{1/2}$. The solution of this is clearly

$$\psi_{\mathbf{n}}(x)=\pi^{-1/4}(n!)^{-1/2}2^{-n/2}H_n(\beta_{\mathbf{n}}^{1/4}x)e^{-(1/2)\beta_{\mathbf{n}}^{1/2}x^2}, \quad (26)$$

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

$$\beta_{\mathbf{n}}=\left(\frac{E}{n+\frac{1}{2}}\right)^2, \quad (27)$$

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 Fig. 1. The orthonormality relation, $\langle\psi_{\mathbf{n}}|\frac{1}{2}x^2|\psi_{\mathbf{n}'}\rangle=N_{\mathbf{n}}\delta_{\mathbf{nn}'}$, then reads

$$\int H_n(\beta_{\mathbf{n}}^{1/4}x)H_{n'}(\beta_{\mathbf{n}'}^{1/4}x)e^{-(1/2)(\beta_{\mathbf{n}}^{1/2}+\beta_{\mathbf{n}'}^{1/2})x^2}x^2dx = N_{\mathbf{n}}\sqrt{\pi}2^{n+1}n!\,\delta_{\mathbf{nn}'}. \quad (28)$$

The first few normalization factors $N_{\mathbf{n}}$ turn out to be as in Table I. We see that $N_{\mathbf{n}}\propto E^{-3/2}$—in general, $\langle\psi_{\mathbf{n}}|x^k|\psi_{\mathbf{n}'}\rangle \propto E^{-(k+1)/2}$ for $k=0,1,2,\ldots$. This is easily seen from a simple scaling argument: perform the scaling $x\rightarrow\beta_{\mathbf{n}}^{1/4}x \sim E^{1/2}x$ (for the sake of this argument we can ignore the n dependence), in the integral and the result follows directly.

From Table I it is clear that

$$N_n=\frac{(2n+1)^{3/2}}{8\sqrt{2}}E^{-3/2}=\frac{1}{4}\beta_{\mathbf{n}}^{-3/4}. \quad (29)$$

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 $T_{\mathbf{nn}'}=\int\psi_{\mathbf{n}}^*\psi_{\mathbf{n}'}dx$ is

$$T=E^{-1/2}\begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{3}\sqrt{\frac{5}{3}} & 0 & \frac{12}{25}\sqrt{\frac{3}{5}} \\ 0 & \sqrt{\frac{3}{2}} & 0 & -\frac{21}{25}\sqrt{\frac{3}{5}} & 0 \\ -\frac{1}{3}\sqrt{\frac{5}{3}} & 0 & \sqrt{\frac{5}{2}} & 0 & -\frac{132}{343}\sqrt{\frac{30}{7}} \\ 0 & -\frac{21}{25}\sqrt{\frac{3}{5}} & 0 & \sqrt{\frac{7}{2}} & 0 \\ \frac{12}{25}\sqrt{\frac{3}{5}} & 0 & -\frac{132}{343}\sqrt{\frac{30}{7}} & 0 & \frac{3}{\sqrt{2}} \end{pmatrix}. \quad (30)$$

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

$$\psi_{\mathbf{n}}=\pi^{-d/4}2^{-dn/2}\left(\prod_{i=1}^{d}(n_i!)^{-1/2}H_{n_i}(\beta_{\mathbf{n}}^{1/4}x_i)\right)e^{-(1/2)\beta_{\mathbf{n}}^{1/2}(x_1^2+\cdots x_d^2)}. \quad (31)$$

Note, $\beta_{\mathbf{n}}=\beta_n$ depends only on $n=n_1+\cdots n_d$, 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 has 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

$$\phi_{\mathbf{n}}(k)=\pi^{-1/4}(n!)^{-1/2}2^{-n/2}\sqrt{\frac{2\pi}{\beta_{\mathbf{n}}^{1/4}}}\left(1+\frac{1}{2}\beta_{\mathbf{n}}^{1/4}\right)H_n\left(ik\left(1+\frac{1}{2}\beta_{\mathbf{n}}^{1/4}\right)^{-1/2}\right)e^{(1/2)k^2\beta_{\mathbf{n}}^{-1/2}} \quad (32)$$

is the Fourier transform of $\psi_{\mathbf{n}}$. The Hermite polynomials of imaginary arguments appear in this formula, this means that for n even $\phi_{\mathbf{n}}$ 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

$$\int H_n\left(ik\left(1+\frac{1}{2}\beta_{\mathbf{n}}^{1/4}\right)^{-1/2}\right)H_{n'}\left(ik\left(1+\frac{1}{2}\beta_{\mathbf{n}'}^{1/4}\right)^{-1/2}\right)e^{(1/2)k^2(\beta_{\mathbf{n}}^{1/2}+\beta_{\mathbf{n}'}^{1/2})}(k^2-2E)dk=-\frac{1}{\sqrt{2\pi}}n!2^{n+1}\beta_{\mathbf{n}}^{5/4}N_{\mathbf{n}}\left(1+\frac{1}{2}\beta_{\mathbf{n}}^{1/4}\right)^{-2}\delta_{\mathbf{nn}'}, \tag{33}$$

a somewhat unexpected result.

IV. ANHARMONIC OSCILLATOR

We now add a new potential $V'=\alpha x^3$ to V, furthermore, to get a feeling of how the Sturmian method works, we will begin by considering the ''standard case'' of $E'=E$—this is what is usually done in the literature. It will turn out, however, that taking $E'\neq E$ is advantageous in our case.

We then need to compute the matrix elements of this in the basis of harmonic oscillator Sturmians. We need to compute the matrix $W^{(3)}_{\mathbf{nn}'}=\int\psi^*_{\mathbf{n}}x^3\psi_{\mathbf{n}'}dx$. For $\mathbf{n},\mathbf{n}'=0,1,\ldots,4$ we obtain the following explicit result:

$$W^{(3)}=E^{-2}\begin{pmatrix} 0 & \frac{27}{64} & 0 & -\frac{343\sqrt{3}}{2048} & 0 \\ \frac{27}{64} & 0 & \frac{7425\sqrt{5}}{2048} & 0 & -\frac{3159}{512\sqrt{2}} \\ 0 & \frac{7425\sqrt{5}}{2048} & 0 & \frac{677425\sqrt{5}}{41472} & 0 \\ -\frac{343\sqrt{3}}{2048} & 0 & \frac{677425\sqrt{5}}{41472} & 0 & \frac{431831169}{4194304} \\ 0 & -\frac{3159}{512\sqrt{2}} & 0 & \frac{431831169}{4194304} & 0 \end{pmatrix}. \tag{34}$$

The secular equation then reads [put $E'=E$ in the general secular equation (7)]

$$\det((1-\beta_{\mathbf{n}})N_{\mathbf{n}}\delta_{\mathbf{nn}'}+\alpha W^{(3)})=0. \tag{35}$$

By including the first N Sturmians we obtain the ground-state energies shown in Table II with $\alpha=0.1$.

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

$$W^{(4)}=E^{-5/2}\begin{pmatrix} \frac{3}{16\sqrt{2}} & 0 & \frac{25}{144}\sqrt{\frac{5}{3}} & 0 & -\frac{243}{1000}\sqrt{\frac{3}{5}} \\ 0 & \frac{135}{16}\sqrt{\frac{3}{2}} & 0 & \frac{27783}{2000}\sqrt{\frac{3}{5}} & 0 \\ \frac{25}{144}\sqrt{\frac{5}{3}} & 0 & \frac{975}{16}\sqrt{\frac{5}{2}} & 0 & \frac{625725}{9604}\sqrt{\frac{15}{14}} \\ 0 & \frac{27783}{2000}\sqrt{\frac{3}{5}} & 0 & \frac{3675}{16}\sqrt{\frac{7}{2}} & 0 \\ -\frac{243}{1000}\sqrt{\frac{3}{5}} & 0 & \frac{625725}{9604}\sqrt{\frac{15}{14}} & 0 & \frac{29889}{16\sqrt{2}} \end{pmatrix}. \tag{36}$$

As for x^3 we obtain the energies E by including the first $N=1,\ldots,5$ Sturmians also shown in Table II. 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 (in their one-center form as well as in their many-center form) where the convergence is very rapid. This failure can be traced back to the nonconvergence of the matrix elements $W^{(k)}_{\mathbf{nn}'}\to\infty$ for $n,n'\to\infty$, which again is a consequence of the divergent behavior of the potentials as $x\to\infty$. Although the Coulomb and Yukawa potentials are singular at the origin, $r=0$, their matrix elements nonetheless fall off rather rapidly as the quantum numbers increase, due to the quick fall off of the potentials themselves as r increases.

But all is not lost yet. The anharmonic oscillator is a very well-studied case precisely because standard techniques tend to fail. We will see that although the Sturmian method gives

TABLE II. The energies for the cubic and quartic anharmonic oscillators $V'=\alpha x^3$ and αx^4, with $\alpha=0.1$ found by using only the first N Sturmians. Only the ground-state energies are shown.

N	$E(x^3)$	$E(x^4)$
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

a nonconvergent series, it is still of great use.

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

$$E_0'=E_0-\frac{11}{8}\frac{\hbar^2\alpha^2}{m^3\omega^4} \quad \text{(cubic potential)}, \tag{37}$$

$$E_0'=E_0+\frac{3}{16}\frac{\hbar^2\alpha}{m^2\omega^2}-\frac{23}{4}\frac{\hbar\alpha^2}{m^2\omega^3} \quad \text{(quartic potential)} \tag{38}$$

by going to second order in the coupling constant α and using standard Rayleigh-Schrödinger perturbation theory, which gives a nonconvergent series—for the particular example of $m=\hbar=\omega=1$ and $\alpha=0.1$ we obtain $E_0'=0.3625$ for the cubic anharmonic oscillator 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 nonperturbative is suggested by the general solution of the secular equation. For the quartic anharmonic potential the ground-state energy as a function of α 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 α 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 behavior of E_0' as a function of the coupling constant α: as α 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 nonperturbative results. The divergence of the perturbation series can be improved in a number of ways, as done recently by Bender and Bettencourt [8], and Kunihiro [9]. The latter author performed a resummation of the perturbation series by using a renormalization-group improved technique. From this, very rapidly converging expressions for the ground-state energy for the quartic anharmonic oscillator are found. Some high-precision numerical results for the quartic anharmonic oscillator were found in Ref. [10], and we will make a comparison with those findings. Other recent papers on related topics are contained in Ref. [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 obtain $\beta_{\mathbf{n}}=1$ (we will say we are ''on shell'') and the secular equation simplifies, since the results then no longer depend on the normalization factor $N_{\mathbf{n}}\propto E^{-3/2}$. Let the number of Sturmians in our basis set be N; then for $N=1$ we obtain simply

$$E'=E+\alpha\frac{\langle\psi_{\mathbf{n}}|x^4|\psi_{\mathbf{n}}\rangle}{\langle\psi_{\mathbf{n}}|\psi_{\mathbf{n}}\rangle}\equiv E+\alpha T_{\mathbf{nn}}^{-1}W_{\mathbf{nn}}^{(4)}. \tag{39}$$

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

$$0=(E-E')^2T_{\mathbf{nn}}T_{\mathbf{n+1,n+1}}+\alpha(E-E')(T_{\mathbf{nn}}W_{\mathbf{n+1,n+1}}^{(4)}+T_{\mathbf{n+1,n+1}}W_{\mathbf{nn}}^{(4)})+\alpha^2W_{\mathbf{nn}}^{(4)}W_{\mathbf{n+1,n+1}}^{(4)}, \tag{40}$$

which, interestingly, can be rewritten as

$$E'=E+\frac{\alpha}{2}\left\{\begin{array}{c}\dfrac{W_{\mathbf{n+1,n+1}}^{(4)}}{T_{\mathbf{nn}}}\\ \dfrac{W_{\mathbf{nn}}^{(4)}}{T_{\mathbf{n+1,n+1}}}\end{array}\right., \tag{41}$$

analogous to Eq. (39).

For $n=0,1,\ldots,4$ we obtain the results shown in Table III, where we also show the highly accurate (approximately 90 significant digits) of Ref. [10]. We note that this crude Sturmian approximation is able to obtain the *right order of*

TABLE III. A comparison between the perturbed energy states for the quartic anharmonic oscillator with $\alpha=0.1$ found by using two Sturmians and the high-precision results of Ref. [10]. The second-order perturbative result for this case ($m=\frac{1}{2}$, $\omega=2$) is $E_0=0.4900$ for the ground state.

	E (Sturmian)		E (Ref. [10])	Difference	
n	$N=1$	$N=2$		$N=1$	$N=2$
0	1.07500	1.07500	1.06529	−0.00971	−0.00971
1	3.37500	3.37500	3.30687	−0.06813	−0.06813
2	5.97500	5.97500	5.74795	−0.22705	−0.22705
3	8.87500	7.00152	8.35268	−0.52232	1.35116
4	12.0750	9.30093	11.09860	−0.97640	1.79767

magnitude for the energy states *even for the excited states*, but we also note that the *accuracy decreases* as n increases. This is once more due to the nonconvergence of the matrix elements of the perturbation potential. Increasing the basis set will *not* lead to an 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, $N=1$. This is in contrast to the case of asymptotically well-behaved potentials such as the Coulomb and Yukawa ones, hitherto studied in the literature.

V. COMMENT ON TIME-DEPENDENT POTENTIALS: THE DAMPED OSCILLATOR

Another important variant of the harmonic oscillator is the damped oscillator. The particular Hamiltonian we are going to study is the so-called Caldirola-Kanai oscillator [12,13],

$$H=\frac{p^2}{2}e^{-2\gamma t}+\frac{1}{2}\omega x^2 e^{2\gamma t}, \tag{42}$$

where γ is some constant, the friction, and t denotes time. This can be re-expressed in terms of a potential V',

$$V'=\frac{1}{2}\omega^2 x^2 e^{2\gamma t'(t)}\equiv\xi(t)V_0(x), \tag{43}$$

with

$$t'(t)=\frac{1-e^{-2\gamma t}}{\gamma}. \tag{44}$$

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

$$(D+V_0+V'(t))\psi=i\hbar\frac{\partial}{\partial t}\psi \tag{45}$$

expanding $\psi=\Sigma_{\mathbf{n}}c_{\mathbf{n}}(t)\psi_{\mathbf{n}}$ leads to the modified secular equation

$$\sum_{\mathbf{n}}\left[(1-\beta_{\mathbf{n}})N_{\mathbf{n}}\delta_{\mathbf{nn}'}+\langle\psi_{\mathbf{n}'}|V'(t)|\psi_{\mathbf{n}}\rangle+E\langle\psi_{\mathbf{n}'}|\psi_{\mathbf{n}}\rangle\right]c_{\mathbf{n}}=i\hbar\sum_{\mathbf{n}}\dot{c}_{\mathbf{n}}\langle\psi_{\mathbf{n}'}|\psi_{\mathbf{n}}\rangle. \tag{46}$$

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

$$\sum_{\mathbf{n}}\left\{\left[1-\beta_{\mathbf{n}}(1+\xi(t))\right]N_{\mathbf{n}}\delta_{\mathbf{nn}'}+E\langle\psi_{\mathbf{n}'}|\psi_{\mathbf{n}}\rangle\right\}c_{\mathbf{n}}=i\hbar\sum_{\mathbf{n}}\dot{c}_{\mathbf{n}}\langle\psi_{\mathbf{n}'}|\psi_{\mathbf{n}}\rangle. \tag{47}$$

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

$$c_{\mathbf{n}}(t)=c_{\mathbf{n}}(0)\exp\left(-it\left[(1-\beta_{\mathbf{n}})\frac{N_{\mathbf{n}}}{T_{\mathbf{nn}}}+E\right]-i(1-\beta_{\mathbf{n}})\frac{N_{\mathbf{n}}}{T_{\mathbf{nn}}}\int_0^t\xi(t')dt'\right). \tag{48}$$

It turns out that one can actually compute the integral. $\xi(t)=e^{2-2e^{-2\gamma t}}$, and the integral can be expressed in terms of the exponential integral function leading to

$$c_{\mathbf{n}}(t)=c_{\mathbf{n}}(0)e^{-i\omega_0 t-i\omega(t)}, \tag{49}$$

where

$$\omega_0=(1-\beta_{\mathbf{n}})\frac{N_{\mathbf{n}}}{T_{\mathbf{nn}}}+E, \tag{50}$$

$$\omega(t)=(1-\beta_{\mathbf{n}})\frac{N_{\mathbf{n}}}{T_{\mathbf{nn}}}\frac{e^2}{2\gamma}(\mathrm{Ei}(-2)-\mathrm{Ei}(-2e^{-2\gamma t})). \tag{51}$$

Naturally, ''on shell'' (i.e., for $\beta_{\mathbf{n}}=1$) we simply obtain $c_{\mathbf{n}}(t)=c_{\mathbf{n}}(0)e^{-iEt}$, as one would expect, whereas ''off shell'' (i.e., for $\beta_{\mathbf{n}}\neq 1$) we obtain a highly oscillatory behavior. The explicit results for $N=1$, $n=0$ are $\omega_0=(1+4E^2)/8E$, $\omega(t)=[e^2(1-4E^2)]/16E\gamma(\mathrm{Ei}(-2)-\mathrm{Ei}(-2e^{-2\gamma t}))$. One should also note that this result holds even for $N\neq 1$; one must then interpret the division by $T_{\mathbf{nn}}$ as multiplication from the left by the inverse $T^{-1}_{\mathbf{nn}'}$, whereby $\omega_0,\omega(t)$ become matrices.

The real and imaginary parts of $c_0(t)\psi_0(x)$ are plotted in Figs. 2(a) and 2(b). We note that the oscillations in the t direction die out either as x increases [because of the decrease of $\psi_0(x)$] or as t does.

The Caldirola-Kanai oscillator can be solved, and the solution is known to be [13] (with $\omega=1$)

$$\phi_n(x)=\frac{1}{\sqrt[4]{\pi}\sqrt{\epsilon}}\left(\frac{\epsilon^*}{2\epsilon}\right)^{n/2}\frac{1}{\sqrt{n!}}\exp\left(\frac{i\dot{\epsilon}e^{2\gamma t}}{2\epsilon}x^2\right)H_n\left(\frac{x}{|\epsilon|}\right),$$

where $\epsilon=\Omega^{-1/2}e^{-(\gamma-i\Omega)t}$, $\Omega=\sqrt{1-\gamma^2}$. This can be rewritten as

$$\phi_n(x)=\sqrt[4]{\frac{1-\gamma^2}{\pi}}e^{1/2\gamma t-[n+(1/2)]i\sqrt{1-\gamma^2}t}2^{-n/2}(n!)^{-1/2}e^{-(1/2)i(\gamma-i\sqrt{1-\gamma^2})e^{2\gamma t}x^2}H_n(\sqrt{1-\gamma^2}e^{\gamma t}x).$$

These states are related to our Sturmians through a rather complicated linear transformation due, essentially, to the Sturmians not being orthonormal with respect to the standard L^2 inner product. Moreover, the states ϕ_n have $\langle H\rangle=0$, which in our case can be achieved by simply letting $E=0$, but, beyond that, it is very difficult to actually compare the two solutions. For $E=n+\frac{1}{2}$, i.e., ''on shell,'' the two expressions for $\langle H\rangle$ differ by a quantity which grows as either γ or t grows. In any case, $c_{\mathbf{n}}(t)\psi_{\mathbf{n}}(t)$ is, by construction, a solution to the time-dependent Schrödinger equation, although the transformation connecting the Sturmians with the exact states ϕ_n is nonunitary (is not an isometry). Furthermore, the Sturmians have the advantage of also being defined for $\gamma\geqslant 1$, whereas ϕ_n is only defined for $0\leqslant\gamma<1$.

This simple example does show, however, 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, which is nice since it is known that the Caldirola-Kanai oscillator can be solved by using a time-dependent canonical transformation on the usual harmonic oscillator [12].

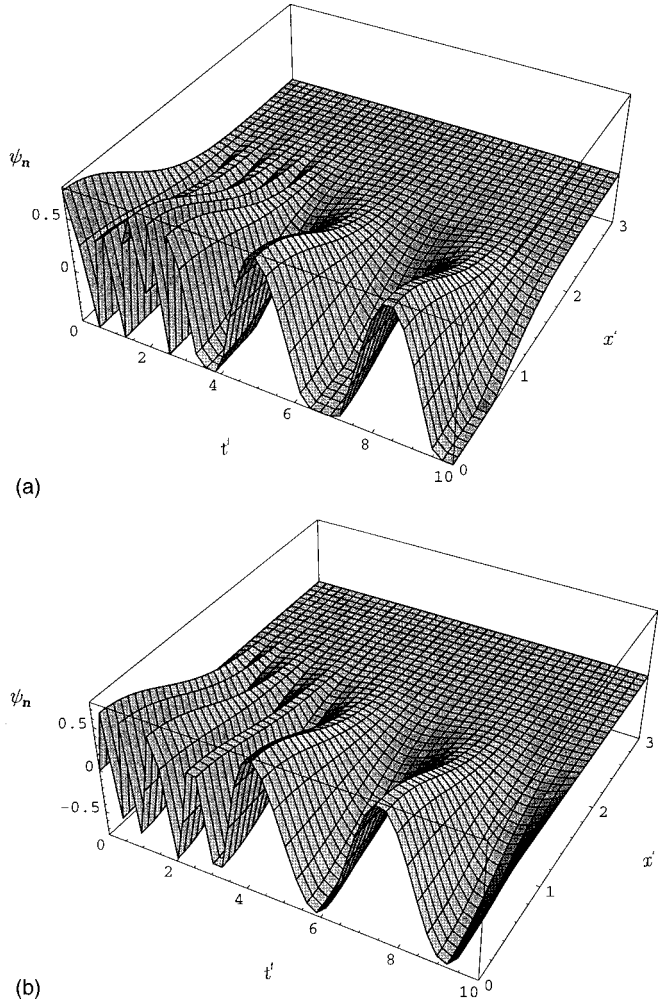

FIG. 2. The real (a) and imaginary (b) parts of the first time-dependent Sturmian for the damped (Caldirola-Kanai) oscillator, $c_n(t)\psi_0(x)$, in the ranges $t\in[0,10]$ and $x\in[0,5]$, and with $E=\gamma=1$.

VI. BATH OF HARMONIC OSCILLATORS

Consider the potential

$$V=\tfrac{1}{2}\sum_i g_i(x-x_i)^2, \tag{52}$$

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 analog of the many-center Coulomb potential treated in Refs. [4,5]. Note that we can rewrite V as

$$V=\tfrac{1}{2}\bar{g}x^2-x\sum_i g_i x_i+\tfrac{1}{2}\sum_i g_i x_i^2 \tag{53}$$

$$\equiv\bar{g}V_0-xc_1+c_2, \tag{54}$$

where $\bar{g}=\Sigma_i g_i$, $c_1=\Sigma_i g_i x_i$, and $c_2=\frac{1}{2}\Sigma_i g_i x_i^2$; 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-center Sturmians introduced for the Coulomb potential in Refs. [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 $V^t(k)$ 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,

$$V=\frac{1}{2}\bar{g}\left(x-\frac{c_1}{2\bar{g}}\right)^2+c_2-\frac{c_1^2}{4\bar{g}}, \tag{55}$$

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

$$x \to x + \frac{c_1}{2\bar{g}}, \quad \beta_{\mathbf{n}} \to \bar{g}\beta_{\mathbf{n}}, \quad E \to E - c_2 + \frac{c_1^2}{4\bar{g}}, \tag{56}$$

i.e., the new $\beta_{\mathbf{n}}$, $\tilde{\beta}_{\mathbf{n}}$, say, reads

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

Hence the Sturmians read

$$\Psi_{\mathbf{n}}(x;x_i) = \pi^{-1/4}(n!)^{-1/2}2^{-n/2}H_n\left(\tilde{\beta}_{\mathbf{n}}^{1/4}\left(x + \frac{c_1^2}{4\bar{g}}\right)\right)e^{-(1/2)\sqrt{\tilde{\beta}_{\mathbf{n}}}[x+(c_1^2)/4\bar{g}]^2}. \tag{57}$$

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

For the many-center Coulomb potential, the Sturmians become related to the one-center Sturmians by means of phase factors $e^{ik_i x_i}$, whereas for the harmonic oscillators the many-center Sturmians are related to the one-center ones by means of a translation $x \to x - c_1^2/4\bar{g}$ 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

$$x \to x + \tfrac{1}{4}(M+1), \quad E \to E - \tfrac{1}{48}M(5M^2+6M+1);$$

thus

$$\tilde{\beta}_{\mathbf{n}} = M\left(\frac{96E - 2M(5M^2+6M+1)}{48(2n+1)}\right)^2,$$

and the first two Sturmians read explicitly

$$\Psi_0(x;x_i) = \pi^{-1/4}\exp\left(-M\frac{48E - M(5M^2+6M+1)}{48}\left(x + \frac{1}{4}(M+1)\right)^2\right), \tag{58}$$

$$\Psi_1(x;x_i) = \pi^{-1/4}\frac{1}{6}\sqrt{M(48E - M(5M^2+6M+1))}\left(x + \frac{1}{4}(M+1)\right)\exp\left(-M\frac{48E - M(5M^2+6M+1)}{144}\left(x + \frac{1}{4}(M+1)\right)^2\right) \tag{59}$$

The energy is found from the Schrödinger equation, which leads to the ''on shell'' condition $\tilde{\beta}_n = 1$. Consequently, the energy of the nth state is

$$E_n = \left(n + \frac{1}{2}\right)\bar{g}^{-1/2} - c_2 + \frac{c_1^2}{4\bar{g}}, \tag{60}$$

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[4]

$$E_n = \left(n + \frac{1}{2}\right)M^{-1/2} - \frac{1}{12}M(M+1)(2M+1) + \frac{1}{16}M(M+1)^2, \tag{61}$$

which is then the energy of a (nonrelativistic) 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.

VII. COMMENT ON COUPLED OSCILLATORS

Consider now a potential of the form

$$V = \tfrac{1}{2}\sum_i g_i(x - x_i)^2 + \tfrac{1}{2}\sum_{i \neq j}\lambda_{ij}(x - x_i)^2(x - x_j)^2, \tag{62}$$

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

$$V = \tfrac{1}{2}\bar{g}x^2 - c_1 x + c_2 - c_3 x^3 + c_4 x^4, \tag{63}$$

where

$$\bar{g} = \sum_i g_i, \tag{64}$$

[4]Note, for $M = 1$, $E \neq n + \frac{1}{2}$, 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 have obtained $V(M=1) = V_0$ and $E(M=1) = n + 1/2$. In that case, by the way, $c_1 = \frac{1}{2}M(M-1)$ and $c_2 = \frac{1}{12}M(M-1)(2M-1)$.

$$c_1=\sum_i 2\left(g_i-\sum_{j\neq i}\lambda_{ij}(x_j^2+x_jx_i)\right)x_i, \tag{65}$$

$$c_2=\frac{1}{2}\sum_i\left(g_i+\sum_{j\neq i}x_j^2\right)x_i^2, \tag{66}$$

$$c_3=\sum_{i\neq j}\lambda_{ij}(x_i+x_j), \tag{67}$$

$$c_4=\frac{1}{2}\sum_{i\neq j}\lambda_{ij}. \tag{68}$$

Suppose χ is a solution to the corresponding Schrödinger equation. We can then expand χ either on the ordinary Sturmians, $\psi_{\mathbf{n}}$, or the Sturmians for a bath of oscillators, $\Psi_{\mathbf{n}}$. If we choose the latter option, we have to complete the squares to obtain the center 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 $\psi_{\mathbf{n}}$, $\chi=\Sigma_{\mathbf{n}}\alpha_{\mathbf{n}}\psi_{\mathbf{n}}$. The secular equation then becomes

$$0=\sum_{\mathbf{n}'}\left[(\beta_{\mathbf{n}}+\overline{g})N_{\mathbf{n}}\delta_{\mathbf{nn}'}-c_1W^{(1)}_{\mathbf{nn}'}+c_2T_{\mathbf{nn}'}-c_3W^{(3)}_{\mathbf{nn}'}-c_4W^{(4)}_{\mathbf{nn}'}\right]\alpha_{\mathbf{n}'}, \tag{69}$$

where

$$W^{(k)}_{\mathbf{nn}'}:=\int\psi^*_{\mathbf{n}}x^k\psi_{\mathbf{n}'}dx \tag{70}$$

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

$$W^{(1)}=E^{-1}\begin{pmatrix} 0 & \frac{3}{8} & 0 & -\frac{21}{128}\sqrt{3} & 0\\ \frac{3}{8} & 0 & \frac{75}{128}\sqrt{3} & 0 & -\frac{81}{64\sqrt{2}}\\ 0 & \frac{75}{128}\sqrt{3} & 0 & \frac{1925}{1728}\sqrt{5} & 0\\ -\frac{21}{128}\sqrt{3} & 0 & \frac{1925}{1728}\sqrt{5} & 0 & \frac{508599}{131072}\\ 0 & -\frac{81}{64\sqrt{2}} & 0 & \frac{508599}{131072} & 0 \end{pmatrix} \tag{71}$$

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

$$(\beta_{\mathbf{n}}+\overline{g})N_{\mathbf{n}}+c_2T_{\mathbf{nn}}-c_4W^{(4)}_{\mathbf{nn}}=0, \tag{72}$$

which is a cubic equation for E; e.g., for $n=0$,

$$\overline{g}-3c_4E+4E^2+16c_2E^3=0,$$

which for the extremely simple case of $\overline{g}=c_2=c_4=1$ 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 $N=2$, $\overline{g}=c_i=1$[5] leads to the solutions $E=-9.91107, -1.51155$ and $E=0.129506\pm i0.435961, 0.537995\pm i1.32394$, which then correspond 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.

VIII. 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 potential, but very slowly converging for potentials diverging for $|x|\to\infty$ such as the anharmonic oscillator. To test this hypothesis, we will now briefly consider a toy model, the anharmonic oscillator damped by a Gaussian $V'=\alpha x^k e^{-x^2}$ where $k=3,4$.[6] Including only the first five Sturmians, we obtain the following matrix elements, $\tilde{W}^{(k)}_{\mathbf{nn}'}$ of V', $k=3,4$:

[5] Which, by the way, is only possible for two coupled oscillators if $x_1=\frac{1}{4}(1\mp\sqrt{1+8\sqrt{14}})$ and $x_2=\frac{1}{2}-x_1$, $g_1=\frac{1}{2}\pm\frac{28175}{110608}\sqrt{1+8\sqrt{14}}$, $g_2=1-g_1$.

[6] One could also consider simply the exponentially damped oscillator $V'=x^ke^{-|x|}$, but, due to the presence of the absolute value, the matrix elements become too complicated.

$$\tilde{W}^{(3)=E^{1/2}} = \begin{pmatrix} 0 & \frac{27}{2(3+4E)^{5/2}} & 0 & -\sqrt{\frac{3}{2}}\frac{343(3+2E)}{2(7+8E)^{7/2}} & 0 \\ \frac{27}{2(3+4E)^{5/2}} & 0 & -\frac{225(15-22E)}{4\sqrt{\frac{1}{6}+\frac{4E}{45}}(15+8E)^3} & 0 & \frac{81(243-324E-52E^2)}{4\sqrt{2+\frac{8}{9}E}(9+4E)^4} \\ 0 & -\frac{225(15-22E)}{4\sqrt{\frac{1}{6}+\frac{4E}{45}}(15+8E)^3} & 0 & \frac{1225(525-940E+316E^2)\sqrt{21}}{4\sqrt{1+\frac{12}{35}E}(35+12E)^4} & 0 \\ -\sqrt{\frac{3}{2}}\frac{343(3+2E)}{2(7+8E)^{7/2}} & 0 & \frac{1225(525-940E+316E^2)\sqrt{21}}{4\sqrt{1+\frac{12}{35}E}(35+12E)^4} & 0 & -\frac{250047(107163-207522E+94356E^2-13816E^3)}{8(63+16E)^{11/2}} \\ 0 & \frac{81(243-324E-52E^2)}{4\sqrt{2+\frac{8}{9}E}(9+4E)^4} & 0 & -\frac{250047(107163-207522E+94356E^2-13816E^3)}{8(63+16E)^{11/2}} & 0 \end{pmatrix} \tag{73}$$

$$\tilde{W}^{(4)} = \begin{pmatrix} \frac{3}{4(1+2E)^{5/2}} & 0 & -\frac{75(5-4E)}{8\sqrt{\frac{1}{2}+\frac{3E}{5}}(5+6E)^3} & 0 & \frac{243(243-160E^2)}{16\sqrt{\frac{3}{2}+\frac{5E}{3}}(9+10E)^4} \\ 0 & \frac{5}{2(1+2E/3)^{7/2}} & 0 & -\frac{19845E(21-4E)}{4\sqrt{\frac{1}{14}+\frac{5}{147}E}(21+10E)^4} & 0 \\ -\frac{75(5-4E)}{8\sqrt{\frac{1}{2}+\frac{3E}{5}}(5+6E)^3} & 0 & \frac{75(25-80E+104E^2)}{8\sqrt{1+\frac{2}{5}E}(5+4E)^4} & 0 & -\frac{2025(273375-899100E+1219680E^2-92288E^3)}{16\sqrt{\frac{1}{3}+\frac{14E}{135}}(45+14E)^5} \\ 0 & -\frac{19845E(21-4E)}{4\sqrt{\frac{1}{14}+\frac{5}{147}E}(21+10E)^4} & 0 & \frac{735E(147-112E+40E^2)}{4\sqrt{1+\frac{2E}{7}}(7+2E)^5} & 0 \\ \frac{243(243-160E^2)}{16\sqrt{\frac{3}{2}+\frac{5E}{3}}(9+10E)^4} & 0 & \frac{2025(273375-899100E+1219680E^2-92288E^3)}{16\sqrt{\frac{1}{3}+\frac{14E}{135}}(45+14E)^5} & 0 & \frac{729(19683-69984E+106272E^2-32256E^3+5248E^4)}{32(9+2E)^{13/2}} \end{pmatrix} \tag{74}$$

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

N	$E(x^3)$	$E(x^4)$
1	0.500000	0.622877
2	0.495852	0.622877
3	0.491822	0.622878
4	0.491282	0.622877
5	0.491282	0.622878

which leads to the ground-state energies shown in Table IV. We notice the improved convergence properties supporting our claim that it was the nonconvergence of the matrix elements of the undamped anharmonic oscillator that was the cause or the nonconvergence of the ground-state energies in the Sturmian method.

IX. 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 nonperturbative, but the divergence of the potential (as $x\rightarrow\pm\infty$) leads to a nonconvergence of the Sturmian approximation, in contrast to the Coulomb case, where we have very rapid convergence. It turned out, however, that already with $N=1$ and 2 Sturmians the correct order of magnitude for the energies of even the excited states could be obtained. This indicates 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 utilize a hybrid method, using the first few Sturmians to obtain the correct order of magnitude and then some variational approach, say, to obtain 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 regularized) potential, convergent at infinity but with the same behavior for x not too large, we did obtain 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. The failure of the numerical approximation to converge for the case of a divergent potential suggests that the Sturmian secular equation should only be taken as defining an *asymptotic expansion* for the energy. This is just like the usual perturbation expansion, but with the important difference that the Sturmian results are nonperturbative, and therefore the first, rough approximation of only using one Sturmian basis function gives considerably better accuracy than finite-order perturbation theory. This is certainly an interesting possibility, but to answer it satisfactorily one would probably have to make a thorough study based on the renormalization-group and/or on partial resummation techniques, which would require a paper of its own.

Given the generality of the approach, as outlined in Sec. I, the Sturmian procedure should also be extendible, for instance, to problems in quantum field theory using a functional Schrödinger picture, and to problems in quantum kinetic theory in phase space using Wigner functions. In field theory the inner product, however, becomes more complicated and a lot of care will have to be taken.

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APPENDIX: CERTAIN RESULTS CONCERNING HERMITE POLYNOMIALS

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

$$e^{-s^2+sx}=\sum_{n=0}^{\infty}\frac{s^n}{n!}H_n(x); \tag{A1}$$

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 require the Fourier transform of a harmonic-oscillator Sturmian. Thus we want to compute the integral

$$\int_{-\infty}^{\infty}e^{ikx}H_n(\alpha x)e^{-(1/2)\beta x^2}dx.$$

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

$$\int e^{-s^2+\alpha sx-(1/2)\beta x^2+ikx}dx$$

$$=e^{-s^2}\sqrt{\frac{2\pi}{\beta}}e^{(1/2\beta)(\alpha s+ik)^{d2}} \tag{A2}$$

$$=\sum_{n=0}^{\infty}\frac{s^n}{n!}\int H_n(\alpha x)e^{-(1/2)\beta x^2+ikx}dx, \tag{A3}$$

from which, by Taylor expansion, we obtain the desired result:

$$\int H_n(\alpha x)e^{-(1/2)\beta x^2+ikx}dx$$

$$=\sqrt{\frac{2\pi}{\beta}}\left(1+\frac{\alpha^2}{2\beta}\right)^{n/2}H_n\left(ik\frac{\alpha}{\beta}(1+\alpha^2/(2\beta))^{-1/2}\right)$$

$$\times e^{(1/2)\beta^{-1}k^2}. \tag{A4}$$

Actually, this formula is a little more general than we need.

For harmonic-oscillator Sturmians it turns out that $\alpha=\beta$ $[=(\beta_{\mathbf{n}}m)^{1/4}]$ which leads to a slight simplification, resulting in the formula given in the text.

Another expression we need is the matrix element of x^γ for γ some positive integer $\geqslant 2$, i.e., we need to compute

$$I_{nm}(\alpha,\beta,\gamma,\delta) := \int H_n(\alpha x)H_m(\beta x)x^\gamma e^{-(1/2)\delta x^2}dx. \tag{A5}$$

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

$$\begin{aligned}
&\int e^{-2s^2+2(\alpha+\beta)sx-(1/2)\delta x^2}x^\gamma dx \\
&\quad = e^{-2s^2}2^{\gamma/2}\delta^{-1-\gamma/2}\Gamma\left(1+\frac{\gamma}{2}\right) \\
&\qquad \times\left(2(\alpha+\beta)s(1-(-1)^\gamma)\ {}_1F_1\right. \\
&\qquad \times\left(1+\frac{\gamma}{2};\frac{3}{2};2\frac{(\alpha+\beta)^2s^2}{\delta}\right) \\
&\qquad +(1+(-1)^\gamma)\sqrt{\frac{\delta\pi}{2}} \\
&\qquad \left.\times\exp\left(2\frac{(\alpha+\beta)^2s^2}{\delta}\right)L_{\gamma/2}^{-1/2}\left(-2\frac{(\alpha+\beta)^2s^2}{\delta}\right)\right)
\end{aligned} \tag{A6}$$

$$\equiv \mathcal{I}(\alpha,\beta,\gamma,\delta), \tag{A7}$$

which is valid even for noninteger γ. Here ${}_1F_1$ is a hypergeometric function, and L_a^b is an associated Laguerre polynomial. The first few of these are

$$L_1^{-1/2}(x)=\tfrac{1}{2}-x,$$

$$L_2^{-1/2}(x)=\tfrac{1}{8}(3-12x+4x^2),$$

$$L_3^{-1/2}(x)=\tfrac{1}{48}(15-90x+60x^2-8x^3),$$

$${}_1F_1(\tfrac{3}{2};\tfrac{3}{2};x)=e^x,$$

$${}_1F_1(\tfrac{5}{2};\tfrac{3}{2};x)=\tfrac{1}{3}e^x(3+2x),$$

$${}_1F_1(\tfrac{7}{2};\tfrac{3}{2};x)=\tfrac{1}{15}e^x(15+20x+4x^2).$$

For the two cases of interest to us, where γ is an even or odd positive integer, we obtain a simpler relation since one of the two terms on the right-hand side will vanish.

For $\gamma=2k$ we arrive at

$$\begin{aligned}
\mathcal{I}(\alpha,\beta,2k,\delta) &= 2^{k+1}e^{-2s^2}\delta^{-1-k}k!\sqrt{\frac{1}{2}\pi\delta} \\
&\quad\times\exp\left(2\frac{(\alpha+\beta)^2s^2}{\delta}\right)L_k^{-1/2}\left(-2\frac{(\alpha+\beta)^2s^2}{\delta}\right),
\end{aligned}$$

whereas for $\gamma=2k+1$ we find

$$\begin{aligned}
\mathcal{I}(\alpha,\beta,2k+1,\delta) &= 2^{k+5/2}e^{-2s^2}\delta^{-k-3/2}\Gamma\left(k+\frac{3}{2}\right) \\
&\quad\times s(\alpha+\beta)\ {}_1F_1\left(k+\frac{3}{2};\frac{3}{2};2\frac{(\alpha+\beta)^2s^2}{\delta}\right).
\end{aligned}$$

Taylor expanding in s, we obtain

$$\begin{aligned}
\mathcal{I}(\alpha,\beta,\gamma,\delta) &\equiv \sum_{n=0}^{\infty}\mathcal{I}_n(\alpha,\beta,\gamma,\delta)\frac{s^n}{n!} \\
&= \sum_{n,m=0}^{\infty}\frac{s^{n+m}}{n!m!}I_{nm}(\alpha,\beta,\gamma,\delta).
\end{aligned} \tag{A8}$$

From this we can obtain relationships between the matrix elements $W_{\mathbf{nn}'}^{(k)}$ for different k's, since $I_{nm}\propto W_{\mathbf{nm}}^{(k)}$ for $\alpha=\beta_{\mathbf{n}}^{1/4}$, $\beta=\beta_{\mathbf{m}}^{1/4}$. For instance, such rules as

$$I_{00}=\mathcal{I}_0,$$

$$I_{01}+I_{10}=\mathcal{I}_1,$$

$$\tfrac{1}{2}I_{02}+\tfrac{1}{2}I_{20}+I_{11}=\tfrac{1}{2}\mathcal{I}_2,$$

$$\tfrac{1}{6}(I_{03}+I_{30})+\tfrac{1}{2}(I_{21}+I_{12})=\tfrac{1}{6}\mathcal{I}_3$$

(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 when γ is not a positive integer, we can use it to obtain the matrix elements of the Coulomb potential between harmonic-oscillator Sturmians.

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