

**SPACE-TIME TRANSFORMATIONS IN RADIAL PATH INTEGRALS**

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Nonlinear space-time transformations in the radial path integral are discussed. A transformation formula is derived, which relates the original path integral to the Green function of a new quantum system with an effective potential containing an observable quantum correction  $\sim \hbar^2$ . As an example the formula is applied to spherical brownian motion.

In recent years Feynman's path integral formulation of quantum mechanics, statistical mechanics and quantum field theory [1,2] has proven a surprisingly powerful method in a large variety of problems reaching from particle physics, atomic physics, solid state physics, polymer physics, stochastic processes to quantum gravity [3,4]. It is, therefore, not exaggerated to say that functional integrals play a similar role in modern theoretical physics as did differential equations in the last centuries. Curiously enough the most important system of quantum mechanics, the hydrogen atom, has resisted a complete path integral treatment for more than three decades. It was only recently that Duru and Kleinert [5] (see also ref. [6]) were able to derive from the path integral the full Feynman kernel of the Coulomb potential. The authors of ref. [5] work with the phase space path integral in cartesian coordinates and transform it into the corresponding path integral of the four-dimensional harmonic oscillator, whose path integral solution is known. This transformation becomes possible by the combined use of a new path-dependent time variable and the Kustaanheimo-Stiefel transformation [7], the latter being a nonlinear mapping from  $\mathbb{R}^3$  to  $\mathbb{R}^4$  known from astronomy.

For three-dimensional quantum systems with spherically symmetric potentials one expects a simple solution to exist in terms of spherical coordinates. In these coordinates the problem is reduced to a study of an effective one-dimensional system, and one is left with the evaluation of the one-dimensional radial path integral. At present, however, it seems rather hopeless to find a direct way for the calculation of non-gaussian path integrals such as the radial path integral for potentials with a Coulomb singularity  $1/r$ .

At this point one should remember that in ordinary calculus one often encounters integrals which can only be evaluated after a clever transformation of integration variables has been employed. It is, therefore, natural to ask whether analogous transformations can be performed in path integrals such that complicated path integrals are transformed into simpler ones.

In this note I derive the transformation formula for a large class of nonlinear transformations in the radial path integral. Our main result is a new relation between the time-independent radial kernel of a given potential  $V(r)$  and the time-dependent radial kernel of a new quantum system with potential  $W(r)$  - the new potential being uniquely determined by a given transformation. As to applications, the idea is to find a transformation such that the new potential  $W$  possesses a path integral whose solution is known.

A careful treatment of the path integral using Feynman's time lattice subdivision process reveals that the lagrangian of the new quantum system contains a quantum correction proportional to  $\hbar^2$ , which modifies the centrifugal barrier. This additional term is missed in a straightforward transformation of the classical action integral, and is a direct consequence of the stochastic nature of the Feynman paths, which are "continuous but possess no derivative" [1]. Quantum corrections of this type have been discovered at several times (references will be given below).

in particular in connection with the operator ordering problem and the quantization in a riemannian manifold, but since they are of order  $\hbar^2$ , some people have doubted that such terms would be experimentally observable (ref. [3] p. 217). In the relation derived below the quantum correction has a direct physical meaning, since it determines the behaviour of the wavefunction at the origin.

As a simple application and consistency check of our relation, we use it to compute the Feynman kernel of a free particle and (in imaginary time) of spherical brownian motion (Bessel process).

We consider three-dimensional quantum systems described by the Hamiltonian  $H = p^2/2 + V$  with spherically symmetric potentials  $V = V(r)$  ( $\hbar = m = 1$ ). In spherical coordinates  $r, \theta, \phi$ , the Feynman kernel  $K$ , which determines the time evolution of the system from "state a" to "state b", can be expanded into "partial waves" [ $T = t_b - t_a, \cos \theta = \cos \theta_b \cos \theta_a + \sin \theta_a \sin \theta_b \cos(\phi_b - \phi_a)$ ]

$$K(t_b, \mathbf{x}_b; t_a, \mathbf{x}_a | V) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi r_b r_a} K_l(T; r_b, r_a | V) P_l(\cos \theta), \tag{1}$$

where the radial kernel  $K_l$  (with fixed angular momentum  $l$ ) is given by the following *radial path integral* [8--10]

$$\begin{aligned} K_l(T; r_b, r_a | V) &= \int_{r(0)=r_a}^{r(T)=r_b} Dr(t) \exp\left(i \int_0^T dt \left[\frac{1}{2} \dot{r}^2 - l(l+1)/2r^2 - V(r)\right]\right) \\ &= \lim_{N \rightarrow \infty} (2\pi i \epsilon)^{-N/2} \int_0^{\infty} \prod_{k=1}^{N-1} dr_k \exp\left(i \sum_{k=1}^N [\delta_k^2/2\epsilon - \epsilon l(l+1)/2r_k r_{k-1} - \epsilon V(r_k)]\right). \end{aligned} \tag{2}$$

Here the path integral has been defined as the continuum limit of a time lattice with lattice constant  $\epsilon = T/N$ ,  $T$  fixed, and  $r_k = r(t_k), t_k = k\epsilon, r(0) = r_a, r(T) = r_b, \delta_k = r_k - r_{k-1}$ . The kernel  $K_l$  vanishes for  $T < 0$ , is symmetric with respect to  $r_b, r_a$ , and is a solution of the inhomogeneous radial Schrödinger equation

$$[i\partial/\partial t_b + \frac{1}{2}\partial^2/\partial r_b^2 - l(l+1)/2r_b^2 - V(r_b)]K_l(T; r_b, r_a | V) = i\delta(T)\delta(r_b - r_a), \tag{3}$$

with the initial condition

$$\lim_{T \rightarrow 0^+} K_l(T; r_b, r_a | V) = \delta(r_b - r_a). \tag{4}$$

In the following we study the combined transformations  $t \rightarrow \tau, r \rightarrow R$  in the path integral (2), where the new path-dependent "time"  $\tau = \tau(t; r(t))$  [5] and the new radial variable  $R = R(\tau)$  have to be determined from the equations ( $\tau(0; r_a) = 0$ )

$$d\tau = dt/f(r), \quad r = g(R), \tag{5}$$

with suitable real, positive functions  $f$  and  $g$ . Let us assume that the constraint

$$\int_0^{\tau_b} d\tau f(g(R(\tau))) = T \tag{6}$$

has for all admissible paths a unique solution  $\tau_b \geq 0$ . Of course, since  $T$  is fixed, the "time"  $\tau_b$  will be path dependent. In order to incorporate the constraint (6), we insert the identity

$$\begin{aligned}
 & [f(r_b)f(r_a)]^{1/2} \int_0^\infty d\tau_b \delta\left(\int_0^{\tau_b} d\tau f(g(R(\tau))) - T\right) \\
 &= [f(r_b)f(r_a)]^{1/2} \int_{-\infty}^\infty \frac{dE}{d\pi} e^{-iET} \int_0^\infty d\tau_b \exp\left(i \int_0^{\tau_b} d\tau f(g(R))E\right)
 \end{aligned} \tag{7}$$

under the path integral (2).

Let us forget for a moment the stochastic nature of the path integral (2). We then obtain for (2), after employing (5) and (7)  $[g(R_a) = r_a, g(R_b) = r_b, g' = dg(R)/dR, \dot{R} = dR(\tau)/d\tau]$ .

$$N(r_b, r_a) \int_{-\infty}^\infty \frac{dE}{2\pi} e^{iET} \int_0^\infty d\tau_b \int_{R(0)=R_a}^{R(\tau_b)=R_b} DR(\tau) \exp\left[i \int_0^{\tau_b} d\tau \left(\frac{\dot{R}^2}{2} \frac{g'^2}{f(g)} - \frac{l(l+1)}{2} \frac{f(g)}{g^2} - f(g)[V(g) - E]\right)\right] \tag{8}$$

$[N$  is a normalization proportional to the jacobian of the transformation (5)]. If  $f$  and  $g$  fulfill the additional constraints ( $a = \text{const}$ )

$$g'(R)^2/f(g(R)) = 1, \quad f(g(R))/g^2(R) = a/R^2, \quad \forall R \in (0, \infty). \tag{9}$$

it is clear that the transformed path integral (8) can be identified with the radial kernel  $K_l(\tau_b; R_b, R_a | W)$  of a new quantum system with angular momentum  $l'$  (defined by  $l'(l' + 1) = l(l + 1)a$ ) and potential

$$W(R) = f(g(R))[V(g(R)) - E]. \tag{10}$$

For a given potential  $V(r)$  it may be possible to find functions  $f$  and  $g$  [satisfying (5) and (9)] such that for the new potential  $W(R)$  the path integration (8) can be carried out.

After this heuristic discussion, we have to investigate the transformation more carefully. To this end it is convenient to make a specific ansatz for the functions  $f$  and  $g$ . Since we are mainly interested in potentials of the form  $V(r) \sim r^b, b \in \mathbb{R}$ , eq. (10) suggests that functions  $f$  and  $g$  can be chosen with similar form. We are thus led to the simple ansatz

$$f(r) = A_\nu r^\nu, \quad g(R) = R^\mu, \quad \nu, \mu \in \mathbb{R}. \tag{11}$$

The constraints (9) are fulfilled, if we set <sup>†1</sup>

$$\mu = 2/(2 - \nu), \quad A_\nu = 4/(2 - \nu)^2, \quad a = A_\nu, \quad \nu < 2. \tag{12}$$

which leads according to (10) to the *new potential*

$$W_\nu(R) = [4/(2 - \nu)^2] R^{2\nu/(2 - \nu)} [V(R^{2/(2 - \nu)}) - E]. \tag{13}$$

Having defined by eqs. (5), (11) and (12) a class of transformations in the continuum limit, we must specify a corresponding lattice version, which enables us to apply the transformation in the lattice definition of the path integral (2). If the lattice variables on the new lattice are defined by  $r_k = g(R_k), R_k = R(\tau_k)$ , it follows from (5) that the new lattice "constant",  $\epsilon'_k$ , is now  $k$  dependent. A discrete version of (5), (11), which preserves the symmetry of the Feynman kernel, is given by

$$\epsilon'_k = \epsilon [f(g(R_k))f(g(R_{k-1}))]^{-1/2} = \epsilon A_\nu^{-1} (R_k R_{k-1})^{-\nu/(2 - \nu)}. \tag{14}$$

This leads to the following transformation formula for the measure  $D\mathbf{r}$  in path space

<sup>†1</sup> Actually, eqs. (11), (12) with  $\nu \neq 2$  represent the complete solution of (9). In the following we restrict the discussion to the case  $\nu < 2$ .

$$(2\pi i \epsilon)^{-N/2} \prod_{k=1}^{N-1} dr_k = A_\nu^{-1/2} (R_b R_a)^{-\nu/2(2-\nu)} \prod_{k=1}^N (2\pi i \epsilon'_k)^{1/2} \prod_{k=1}^{N-1} dR_k ,$$

i.e.

$$Dr(t) = A_\nu^{-1/2} (r_b r_a)^{-\nu/4} DR(\tau) , \tag{15}$$

where  $DR$  has now the same meaning as  $Dr$  (apart from  $\epsilon \rightarrow \epsilon'_k$ ). From (15) and (7) we deduce for the normalization  $N$  in (8)

$$N(r_b, r_a) = [2/(2-\nu)](r_b r_a)^{\nu/4} . \tag{16}$$

It remains to study the transformation of the lattice action in eq. (2). It is not difficult to see that the centrifugal and potential terms in (2) transform into the corresponding terms of eq. (8). The only term which requires a more careful treatment, is the kinetic energy term  $\delta_k^2/\epsilon$ . Indeed, it is well known that under the path integral  $\delta_k^2$  is of order  $\sqrt{\epsilon}$ , i.e.  $\delta_k^2/\epsilon$  diverges as  $\epsilon \rightarrow 0$ . "The important paths are, therefore, continuous but possess no derivative" [1]. Keeping this in mind, it is obvious from the expansion ( $\Delta_k = R_k - R_{k-1}$ )

$$\delta_k^2/\epsilon = \Delta_k^2/\epsilon'_k + [\nu(4-\nu)/12(2-\nu)^2 R_k R_{k-1}] \Delta_k^4/\epsilon'_k + O(\Delta_k^5/\epsilon'_k) , \tag{17}$$

that the  $\Delta_k^4$  term cannot be neglected as we did in the heuristic derivation of eq. (8). The importance of such terms has already been stressed by Feynman in his basic paper [1]. As an example he discussed a hamiltonian with a vector potential. A general analysis of the relationship between the distance and time differentials in the case of riemannian coordinates was carried out by De Witt [11]. For the free Feynman kernel in polar coordinates the relevance of the fourth order terms was pointed out by Edwards and Gulyaev [8]. McLaughlin and Schulman [12] showed that the unpleasant higher order terms can be eliminated in favor of an effective potential. Gervais and Jevicki [13] nicely illustrated how such terms contribute to two- and higher-loop calculations in Feynman diagrams (see also ref. [14]). In the mathematical formulation of brownian motion, Itô was led to the definition of the so-called stochastic integrals [15]. Without going into mathematical details, the result of all these investigations (relevant to our discussion) may be stated in the following relation

$$\exp \left\{ i \left[ \frac{\Delta_k^2}{2\epsilon'_k} + \frac{\nu(4-\nu)}{24(2-\nu)^2 R_k R_{k-1}} \frac{\Delta_k^4}{\epsilon'_k} + O\left(\frac{\Delta_k^5}{\epsilon'_k}\right) \right] \right\} \doteq \exp \left[ i \left( \frac{\Delta_k^2}{2\epsilon'_k} - \epsilon'_k \frac{\nu(4-\nu)}{8(2-\nu)^2 R_k R_{k-1}} \right) \right] , \tag{18}$$

where the symbol  $\doteq$  denotes equivalence as far as use in the path integral is concerned. Thus the additional term in the radial action amounts to a correction to the centrifugal potential, which added to the centrifugal term in (8) leads to an *effective angular momentum*  $L_\nu$  defined by  $L_\nu(L_\nu + 1) = l(l+1)A_\nu + \nu(4-\nu)(2-\nu)^{-2}/4$ . With (12) one obtains

$$L_\nu = (4l + \nu)/2(2-\nu) . \tag{19}$$

Inserting the correction term in eq. (8), we observe that the path integral in (8) is precisely the path integral representation of the radial kernel  $K_{L_\nu}(\tau_b, R_b, R_a | W_\nu)$ , where  $W_\nu$  and  $L_\nu$  are given in eqs. (13) and (19), respectively. From (8) and (16) we then obtain for the transformation of the path integral (2)

$$K_l(T; r_b, r_a | V) = [2/(2-\nu)](r_b r_a)^{\nu/4} \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{-iET} \int_0^\infty d\tau_b K_{L_\nu}(\tau_b; R_b, R_a | W_\nu) . \tag{20}$$

If the time-independent radial kernel  $k_l$  is defined by <sup>†2</sup>

<sup>†2</sup> A small positive imaginary part has to be added to  $E$ .

$$k_l(E; r_b, r_a | V) = i \int_0^\infty dT e^{iET} K_l(T; r_b, r_a | V). \tag{21}$$

we immediately obtain from (20) the transformation formula ( $\nu < 2$ )

$$k_l(E; r_b, r_a | V) = [2i/(2 - \nu)] (r_b r_a)^{\nu/4} \int_0^\infty d\tau_b K_{L_\nu}(\tau_b; r_b^{1-\nu/2}, r_a^{1-\nu/2} | W_\nu). \tag{22}$$

This is the main result of this paper. A few comments are in order:

(i) For  $\nu = 0$ , the transformation (5) combined with (11) and (12) is the identity transformation. This is consistent with eq. (22), since in this case one obtains  $W_0(R) = V(R) - E$ ,  $L_0 = l$ , and the  $E$  dependence of the kernel  $K_{L_0}$  completely factorizes,  $K_{L_0}( | W_0) = \exp(iE\tau_b) K_l( | V)$ .

(ii) In the above derivation we assumed that the time integral in (22) exists. If the quantum system belonging to the new potential  $W_\nu$  possesses zero modes, they must be properly subtracted.

(iii) Relation (22) enables us to express the Feynman kernel of a given potential  $V$  with fixed angular momentum  $l$  by the Feynman kernel of a new potential  $W_\nu$  with effective angular momentum  $L_\nu$ . The energy dependence of the l.h.s. of (22) appears as a "coupling constant" dependence on the r.h.s. via the second term in the potential (13).

(iv) The effective angular momentum  $L_\nu$ , eq. (19), is in general not an integer. The radial kernel on the r.h.s. of (22) has, therefore, to be understood as the analytic continuation from physical  $l$  values to the  $L_\nu$  values implied by (19). From Regge theory we know that this analytic continuation is always possible for  $\text{Re } L_\nu > -1/2$ . This condition implies (for  $\nu$  real  $< 2$ )  $\text{Re } l > -1/2$ , which is always fulfilled.

(v) If the Schrödinger wavefunctions are written in the form  $\psi(r, \theta, \phi) = r^{-1} \chi_{ln}(r) Y_l^m(\theta, \phi)$ , the kernels  $K_l$  and  $k_l$  have the spectral decompositions (for simplicity we assume that the system has only a discrete spectrum)

$$K_l(T; r_b, r_a | V) = \sum_n \chi_{ln}(r_b) \chi_{ln}(r_a) \exp(-iE_{ln}T) \Theta(T). \tag{23a}$$

$$k_l(E; r_b, r_a | V) = \sum_n \frac{\chi_{ln}(r_b) \chi_{ln}(r_a)}{E_{ln} - E}. \tag{23b}$$

Here  $n$  denotes the radial quantum number, and  $E_{ln}$  are the energy levels of the system. From Regge theory<sup>3</sup>  $\chi_{ln}(r) \sim r^{l+1}$  for  $r \rightarrow 0$ ,  $\text{Re } l > -1/2$ , which implies for both kernels in (23) the "threshold behaviour"  $r_b^{l+1}$  for  $r_b \rightarrow 0$ ,  $r_a \neq 0$  (with an analogous behaviour in  $r_a$ ). Thus the r.h.s. of (22) behaves for  $r_b \rightarrow 0$ ,  $r_a \neq 0$  as  $r_b^\lambda$  with  $\lambda = \nu/4 + (1 - \nu/2)(L_\nu + 1) = l + 1$  consistent with the l.h.s. of (22). This demonstrates clearly the crucial role played by the additional potential term caused by the stochastic nature of the functional integral. Without this quantum correction the threshold behaviour would be violated with direct experimental consequences.

(vi) If for a given potential  $V$  a transformation has been found for which the r.h.s. of (22) can be calculated as a function of  $E$ , the energy levels and wavefunctions of the original system can be obtained according to eq. (23b) by determining the poles and residues in the energy plane.

(vii) If we define the radial Green function  $G_l$  by

$$G_l(r_b, r_a | V) = i \int_0^\infty dT K_l(T; r_b, r_a | V) = \lim_{E \rightarrow 0} k_l(E; r_b, r_a | V), \tag{24}$$

the transformation formula (22) can be written in the compact form ( $\nu < 2$ )

$$k_l(E; r_b, r_a | V) = [2/(2 - \nu)] (r_b r_a)^{\nu/4} G_{L_\nu}(r_b^{1-\nu/2}, r_a^{1-\nu/2} | W_\nu). \tag{25}$$

As a simple application of relation (25), which will serve the purpose of a consistency check, we put  $V(r) \equiv 0$ ,  $\nu = 1$ ,  $E = k^2/2 > 0$ , and obtain with (19) for the free particle kernel  $k_1^0$  the relation

<sup>3</sup> For potentials with  $\lim_{r \rightarrow 0} r^2 V(r) = 0$ .

$$k_l^0(E; r_b, r_a) = 2(r_b r_a)^{1/4} G_{2l+1/2}^{\text{osc}}(\sqrt{r_b}, \sqrt{r_a}). \tag{26}$$

On the r.h.s. appears the radial Green function of a harmonic oscillator (osc) with purely imaginary frequency  $\Omega = 2ik$ . Indeed, the new potential (13) becomes in this case the harmonic oscillator potential  $W_1(R) = -4ER^2 \equiv \Omega^2 R^2/2$ . The path integration for the harmonic oscillator with real frequency  $\omega$  can be carried out with the result [9]

$$K_l^{\text{osc}}(T; r_b, r_a) = (-i)^{l+3/2} (\sin \omega T)^{-1} \omega \sqrt{r_b r_a} \exp[\frac{1}{2}i\omega(r_b^2 + r_a^2) \cot \omega T] J_{l+1/2}(\omega r_b r_a / \sin \omega T) \Theta(T) \tag{27}$$

( $J_{l+1/2}$  is the Bessel function). Making the necessary analytic continuations in (27) and inserting the result in (22) we obtain ( $k = \sqrt{2E}$ ,  $r_b \geq r_a$ )

$$k_l^0(E; r_b, r_a) = 2i(-1)^{l+1} \sqrt{r_b r_a} \int_0^\infty \frac{dx}{\sinh x} \exp[ik(r_b + r_a) \coth x] J_{2l+1}(2k\sqrt{r_b r_a} / \sinh x) \\ = i\pi \sqrt{r_b r_a} H_{l+1/2}^{(1)}(\sqrt{2E}r_b) J_{l+1/2}(\sqrt{2E}r_a). \tag{28}$$

It is well known that the path integral (2) (with  $V = 0$ ), analytically continued to imaginary time,  $T \rightarrow -it$  ( $t$  real), describes the distribution function of a particle undergoing brownian motion (BM) with diffusion constant  $D = 1/2$ . In this case eq. (21) becomes a Laplace transformation (with  $E \rightarrow -\alpha$ ). Denote the Laplace transform of the distribution function by  $\rho_l(\alpha; r_b, r_a)$ . Then  $\rho_l$  is given by (26) but with a real oscillator frequency  $\Omega_{\text{BM}} = -2\sqrt{2\alpha}$ . (This follows from the observation that the motion of the oscillator in imaginary time takes place in a "mirror potential"  $-W_1(R) = 4\alpha R^2 \equiv \Omega_{\text{BM}}^2 R^2/2$ ). Thus  $\rho_l$  is given by (28), analytically continued to the point  $\sqrt{2E} = i\sqrt{2\alpha}$ . We then obtain in terms of modified Bessel functions (see p. 952 in ref. [16]) ( $r_b \geq r_a$ )

$$\rho_l(\alpha; r_b, r_a) = 2\sqrt{r_b r_a} K_{l+1/2}(\sqrt{2\alpha}r_b) I_{l+1/2}(\sqrt{2\alpha}r_a). \tag{29}$$

This result agrees with the known expression for spherical brownian motion (the Bessel process in three dimensions) [17]<sup>†5</sup>.

Returning to (28), we notice that we can rewrite this equation in the form (see p. 957 in ref. [16])

$$k_l^0(E; r_b, r_a) = i \int_0^\infty dt e^{iET} \{ \sqrt{r_b r_a} (-i)^{l+3/2} T^{-1} \exp[(i/2T)(r_b^2 + r_a^2)] J_{l+1/2}(r_b r_a / T) \}.$$

A comparison with (21) yields the time-dependent radial kernel

$$K_l^0(T; r_b, r_a) = \sqrt{r_b r_a} (-i)^{l+3/2} T^{-1} \exp[(i/2T)(r_b^2 + r_a^2)] J_{l+1/2}(r_b r_a / T) \Theta(T). \tag{30}$$

Inserting the radial kernel (30) in the partial wave expansion (1) we obtain the standard result for the Feynman kernel of a free particle

$$K^0(t_b, \mathbf{x}_b; t_a, \mathbf{x}_a) = (2\pi i T)^{-3/2} \exp[(i/2T)(\mathbf{x}_b - \mathbf{x}_a)^2] \Theta(T), \tag{31}$$

This completes our check of relation (26). Notice that eq. (26) read in the opposite direction leads to the surprising result, that the Green function of the harmonic oscillator can be computed from an analytic continuation of the free particle kernel.

In a second paper we shall illustrate the full power of relation (25) by applying it to the Coulomb potential. As a result we shall determine in a few lines the energy spectrum and the complete normalized wavefunctions of the

<sup>†4</sup> After the substitution  $x = \ln \coth(y/2)$  the integral in (28) can be found on p. 729 in ref. [16], where the result is given in terms of Whittaker functions. The latter have been expressed in terms of Hankel and Bessel functions, respectively, with the help of the relations given on p. 1062 and p. 952 in ref. [16].

<sup>†5</sup> In the notation of ref. [17] we have  $G^H(\alpha, \xi, \eta) = (2\xi\eta)^{-1} \rho_H(\alpha; \eta, \xi)$ .

hydrogen atom. Another application will be the computation of the Green functions of the sextic anharmonic oscillator and the linearly confining potential  $V(r) = \kappa r$ .

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