Coupling-constant behavior of the resonances of the cubic anharmonic oscillator

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Asymptotic formulas for the resonances of the cubic anharmonic oscillator in both the regimes of small and large coupling constant g are derived. In addition, a numerical calculation is carried out to give a complete graphical picture of the behavior of the resonance eigenvalues over the whole range of g.

I. INTRODUCTION

The aim of this paper is to present three results about the cubic anharmonic oscillator

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}kx^2+gx^3 , \tag{1}$$

a standard textbook example of the simplest perturbation to the harmonic oscillator.[1] These are, with k taken equal to 1 and with n the usual harmonic-oscillator quantum number, (i) the asymptotic expansion for the imaginary part of the resonances in the regime of small coupling constant:

$$\operatorname{Im}E_n(g)\sim -i\frac{2^{3n}}{n!\sqrt{\pi}}g^{-(2n+1)}e^{-2/15g^2}\sum_{M=0}^{\infty}b_n^{(M)}g^M \quad \text{as } g\to 0 , \tag{2}$$

(ii) the asymptotic form for the Rayleigh-Schrödinger perturbation theory (RSPT) coefficients:

$$E_n(g)\sim \sum_{N=0}^{\infty}E_n^{(N)}g^N \quad \text{as } g\to 0 , \tag{3}$$

$$E_n^{(N)}\sim -\frac{(60)^{N/2+n+1/2}}{n!(2\pi)^{3/2}2^{3N/2}}\Gamma(\tfrac{1}{2}N+n+\tfrac{1}{2})\left[1+\frac{c_n^{(1)}}{N/2+n-\frac{1}{2}}+\frac{c_n^{(2)}}{(N/2+n-\frac{1}{2})(N/2+n-\frac{3}{2})}+\cdots\right] \quad \text{as } N\to\infty , \tag{4}$$

and (iii) the asymptotic form of the resonances in the regime of large coupling constant:

$$E_n(g)\sim \tfrac{1}{2}e^{-i\pi/5}\left[\frac{5\pi^{3/2}(2n+1)}{\sqrt{3}\Gamma(\frac{1}{3})\Gamma(\frac{1}{6})}\right]^{6/5}(2g)^{2/5} \quad \text{as } g\to\infty . \tag{5}$$

The well-known intuitive conjecture is that under the cubic perturbation the bound states of the harmonic oscillator will become resonances: the particle, initially confined in the potential well, will escape to $x=-\infty$ by tunneling. Mathematically, the problem is more complicated[2-4] because the potential goes to $-\infty$ so strongly. The essential result, given by Caliceti, Graffi, and Maioli,[5] is that if the coupling constant is complex, for $\operatorname{Im}g\neq 0$ the operator (1) has nonempty discrete spectrum (i.e., isolated eigenvalues of finite multiplicity). All these eigenvalues can be analytically continued to $\operatorname{Im}g=0$ and are in one-to-one relation to the solutions (with complex E) of the differential equation

$$-\tfrac{1}{2}\varphi''+(\tfrac{1}{2}kx^2+gx^3)\varphi=E\varphi , \tag{6}$$

with the Gamow-Siegert[6] (i.e., purely outgoing wave) boundary condition at $x=-\infty$. The conclusion is that for the cubic anharmonic oscillator there is a natural concept of resonances: it has been proved[7] that these resonances are limits of resonances in the structural sense of dilation analyticity obtained by any suitable analytic regularization of the potential which makes it classically complete at $x=-\infty$. Furthermore,[5] the RSPT series is Borel summable to the resonance eigenvalues.

In Secs. II and III the analytic derivations of the asymptotic formulas (2)–(5) are discussed. In Sec. IV numerical calculations are carried out to provide a complete graphical picture of the behavior of $E(g)$ over the whole range of values of the coupling constant.

II. SMALL COUPLING-CONSTANT ASYMPTOTICS

A convenient way to obtain the asymptotic expansion for the imaginary part of the resonance eigenvalues is to use a current-density-type formula. Recalling briefly the main steps, let φ denote the resonant wave function. Multiply Eq. (6) by φ^*, subtract the complex conjugate equation, and integrate to show that

$$\operatorname{Im}E(g)=\frac{i}{4}\frac{\varphi^*\dfrac{d\varphi}{dx}-\varphi\dfrac{d\varphi^*}{dx}}{\displaystyle\int_x^{\infty}\varphi^*\varphi\,dx} , \tag{7}$$

an equality which is valid for any finite x, since the resonance wave function vanishes sufficiently fast at $x=+\infty$. The numerator in Eq. (7) is the wronskian of two functions which solve the same differential equation except for the sign of ImE, which turns out to be exponentially small [Eq. (2)]. To estimate the integral in the denominator, let x be a point inside the tunneling region, and write

$$z=4g^2x^2\,, \tag{8}$$

$$\varphi(x)=\left[\frac{4g^2}{z}\right]^{1/4}(-\dot{S}(z))^{-1/2}\exp(S(z)/8g^2)\,, \tag{9}$$

where the dot denotes d/dz. Through the standard Jeffreys-Wentzel-Kramers-Brillouin (JWKB) formulas,[8] this solution connects with the purely outgoing wave at $x=-\infty$. The "normalization factor" $(4g^2)^{1/4}$ makes the numerator of (7) (which can be directly evaluated in the oscillatory region) equal to $2i$ plus exponentially small terms.[9] The corresponding equation for S, which follows from Eqs. (6) and (9) is

$$\tfrac{1}{2}(\dot{S})^2=\tfrac{1}{2}(1-z^{1/2})-g^2\frac{4E}{z}-g^4\frac{6}{z^2}$$

$$-g^2 32(-\dot{S})^{1/2}\frac{d^2}{dz^2}(-\dot{S})^{-1/2}\,. \tag{10}$$

This transformation of independent and dependent variables fixes the zeroth-order turning point at $z=1$ and allows an expansion

$$S(z)\sim\sum_{N=0}^{\infty}S^{(2N)}(z)(2g)^{2N}\,, \tag{11}$$

$$E\sim\sum_{N=0}^{\infty}E^{(2N)}g^{2N}\,, \tag{12}$$

which can be solved recursively in closed form for the $S^{(2N)}$ in terms of elementary functions. Denote

$$y=\sqrt{1-z^{1/2}}\,. \tag{13}$$

Then, the lowest orders are

$$S^{(0)}=\tfrac{4}{3}y^3-\tfrac{4}{5}y^5\,, \tag{14}$$

$$S^{(2)}=2E^{(0)}\ln\left[\frac{1-y}{1+y}\right], \tag{15}$$

$$S^{(4)}=[\tfrac{1}{2}E^{(2)}+\tfrac{15}{8}(E^{(0)})^2+\tfrac{7}{32}]\ln\left[\frac{1-y}{1+y}\right]+\frac{5}{24}\frac{1}{y^3}$$

$$+\left[\frac{1}{y-1}+\frac{1}{y+1}\right]\left[\frac{7(E^{(0)})^2}{8}+\frac{5}{32}\right]$$

$$+\left[\frac{1}{(y+1)^2}-\frac{1}{(y-1)^2}\right]\left[\frac{(E^{(0)})^2}{8}+\frac{3}{32}\right]. \tag{16}$$

The $E^{(2N)}$ are determined by imposing the condition that $S^{(2N)}$ with $N>1$ not have a logarithmic singularity at $z=0$. To cancel the coefficient of the logarithmic term in $S^{(4)}$, one must take

$$E^{(2)}=-\tfrac{15}{4}(E^{(0)})^2-\tfrac{7}{16}=-\tfrac{1}{8}(30n^2+30n+11)\,, \tag{17}$$

which is, of course, the second nonzero coefficient of the RSPT series (3). In fact, because of the invariance of the Hamiltonian under the simultaneous substitutions $x\to -x, g\to -g$, all the odd energy coefficients are null. One can also show that the even coefficients $E^{(2N)}$ are polynomials of degree $N+1$ in the quantum number n.

Once the $S^{(2N)}$ have been obtained, the next step is to evaluate the denominator in Eq. (7). A straightforward procedure is to expand the JWKB wave function into RSPT form:

$$\varphi_{\rm JWKB}=g^{-(2n+1)}e^{1/15g^2}x^n e^{-x^2/2}\sum C_i^{(N)}x^i g^N \tag{18}$$

and carry out the integration in Eq. (7) by letting $x\to\infty$, which greatly simplifies the integration while introducing only an exponentially small error. Since Eq. (18) is precisely the RSPT wave function except for a normalization constant, it is easier from a technical point of view to calculate the RSPT wave function $\varphi_{\rm RSPT}$ independently in the "intermediate normalization" and to apply Eq. (7) in the form

$${\rm Im}E(g)\sim\frac{i}{4}\frac{2i}{\int_{-\infty}^{\infty}\varphi^*_{\rm RSPT}\varphi_{\rm RSPT}\,dx}\left|\frac{\varphi_{\rm RSPT}}{\varphi_{\rm JWKB}}\right|^2$$

$$=-\frac{1}{2}\frac{\partial E(g)}{\partial E^{(0)}}\left|\frac{\varphi_{\rm RSPT}}{\varphi_{\rm JWKB}}\right|^2. \tag{19}$$

[The derivative with respect to $E^{(0)}$ applies only to the explicit unperturbed energy that appears as part of the reduced resolvent in the expression of the perturbed energy (3).] A convenient way to calculate the quotient of the asymptotic expansions is to compare the coefficients of x^n in both expansions, that is, only the term $i=0$ in Eq. (18) need be calculated. In such a way one obtains, to order g^2,

$${\rm Im}E_n(g)=-\frac{2^{3n}}{n!\sqrt{\pi}}g^{-(2n+1)}e^{-2/15g^2}$$

$$\times[1+b_n^{(1)}g+b_n^{(2)}g^2+O(g^3)]\,, \tag{20}$$

$$b_n^{(1)}=0\,, \tag{21}$$

$$b_n^{(2)}=-\tfrac{1}{3456}n^6+\tfrac{29}{1152}n^5+\tfrac{655}{1728}n^4-\tfrac{691}{1152}n^3$$

$$-\tfrac{58\,657}{3456}n^2-\tfrac{14\,735}{576}n-\tfrac{169}{16}\,. \tag{22}$$

(In fact, $b_n^{(2M+1)}=0$.)

Through a dispersion relation[10] in g^2, Im$E_n(g)$ gives the large-N asymptotic behavior of the RSPT coefficients, namely,

$$E_n^{(N)} \sim \tfrac{1}{2}\int_0^\infty (g^2)^{-N/2-1}\,\mathrm{Im}E_n(g^2)d(g^2) \tag{23}$$

$$= -\frac{1}{n!(2\pi)^{3/2}}\frac{(60)^{N/2+n+1/2}}{2^{3N/2}}\Gamma(\tfrac{1}{2}N+n+\tfrac{1}{2}) \times\left[1+\frac{2}{15}\frac{b_n^{(2)}}{N/2+n-\frac{1}{2}}+\left[\frac{2}{15}\right]^2\frac{b_n^{(4)}}{(N/2+n-\frac{1}{2})(N/2+n-\frac{3}{2})}+O(N^{-3})\right] \quad \text{as } N\to\infty\ . \tag{24}$$

Thus the Bender-Wu "correction coefficients" $c_n^{(N)}$ of Eq. (4) are given in terms of the coefficients $b_n^{(2N)}$ of the power series factor in $\mathrm{Im}E_n(g)$ by

$$c_n^{(N)} = (\tfrac{2}{15})^N b_n^{(2N)}\ . \tag{25}$$

III. LARGE EIGENVALUES

Upon the real scale transformation $x \to (2g)^{-1/5}x$ the Schrödinger equation (6) is equivalent to

$$f'' - [x^3 + k(2g)^{-4/5}x^2 - 2(2g)^{-2/5}E]f = 0\ . \tag{26}$$

Considering the exponents of $(2g)$ in Eq. (26), it is plausible to simplify the calculation of the large coupling-constant behavior of the resonance eigenvalues by dropping the x^2 term. This is equivalent to letting $k=0$ in Eq. (6). We again use the JWKB method and apply the Dunham formula to lowest order in the complex plane:

$$\oint_c \sqrt{2E-2gx^3}\,dx = (n+\tfrac{1}{2})2\pi\ . \tag{27}$$

The path of integration encircles the two transition points $x_1 = (E/g)^{1/3}$ and $x_2 = (E/g)^{1/3}e^{-2\pi i/3}$, thus connecting the subdominant JWKB solutions in the corresponding regions $|\arg(x)| < \pi/5$ and $|\arg(x+4\pi/5)| < \pi/5$. The result of the integration[11] is precisely Eq. (5). Incidentally, note that the $g^{2/5}$ factor in Eq. (5) is consequence of the simple Symanzik scaling argument which led to Eq. (26).

The rigorous application of the JWKB method to the differential equation (26) has been extensively studied by Sibuya,[12] who proved the following result: if M is a sufficiently large positive number, the eigenvalues of (6) whose absolute value is greater than M are simple and given by

$$E_n = \tfrac{1}{2}e^{-i\pi/5}\left[\frac{(2n+1)\pi}{2K\sin(2\pi/3)}\right]^{6/5}(2g)^{2/5}[1+\nu_n]\ , \tag{28}$$

where

$$K = \int_0^\infty [(t^3+1)^{1/2} - t^{3/2}]dt\ , \tag{29}$$

n takes all sufficiently large positive integers, and

$$\lim_{n\to\infty}\nu_n = 0\ . \tag{30}$$

Evaluation of the integral K then gives Eq. (5). Sibuya's lengthy proof has an interesting feature: it does not rely on stability with respect to the harmonic oscillator. That is to say, it applies to the pure cubic case, asserting the existence of resonances. This result may appear surprising on physical grounds: the linear potential, $V=gx$, does not have resonances, while the more repulsive $V=gx^3$ does.

IV. NUMERICAL ANALYSIS THROUGH COMPLEX DILATION

The numerical computation of the resonances which will permit us to join the eigenvalues in the "perturbation region" to the large-g regime can be carried out with the complex dilation technique. From the unitary group of dilations in $L^2(\mathbb{R})$, with action

$$[U(\theta)f](x) = e^{\theta/2}f(e^\theta x) \tag{31}$$

and infinitesimal generator

$$A = \tfrac{1}{2}(xp+px)\ , \tag{32}$$

the following dilated operator is obtained:

$$U^{-1}(\theta)HU(\theta) = H(\theta) = \tfrac{1}{2}e^{-2\theta}p^2 + \tfrac{1}{2}e^{2\theta}x^2 + e^{3\theta}gx^3\ . \tag{33}$$

This expression, *a priori* defined for θ real, admits analytic continuation to θ complex.[5] From the computational point of view, the essential fact is that for $\mathrm{Im}\theta > 0$, the resonances of (6) appear as θ-independent complex eigenvalues [in a strict sense, i.e., associated with $L^2(\mathbb{R})$ eigenfunctions] of the complex dilated operator (33):

$$H(\theta)\Psi(\theta) = E\Psi(\theta),\quad E = E_r - \tfrac{1}{2}i\Gamma\ . \tag{34}$$

In consequence, there exists the possibility of approximating $\Psi(\theta)$ in finite dimensional subspaces, with techniques resembling those employed for bound-state calculations. The theoretical drawback is the lack of an analog of the min-max principle. The evidence for the relation between the spectrum of $H(\theta)$ and the spectra of its finite dimensional approximations is essentially numerical.

The natural basis is that of harmonic-oscillator wave functions

$$\phi_n(x) = (\sqrt{\pi}2^n n!)^{-1/2}H_n(x)e^{-x^2/2},\quad n=0,1,2,\ldots \tag{35}$$

with $H_n(x)$ the Hermite polynomials. Consider the operators acting in $\mathbb{C}^N$,

$$H_N(\theta) = \langle \phi_j, H(\theta)\phi_i\rangle_{i,j=1,\ldots,N}\ , \tag{36}$$

which are complex symmetric matrices (*not* self-adjoint). The expectation is that their spectra contain (better for increasing N) approximations to the resonances of $H(\theta)$.

An additional problem comes from the fact that the position of the resonances is (locally) independent of θ, whereas this is not true for the eigenvalues of the truncat-

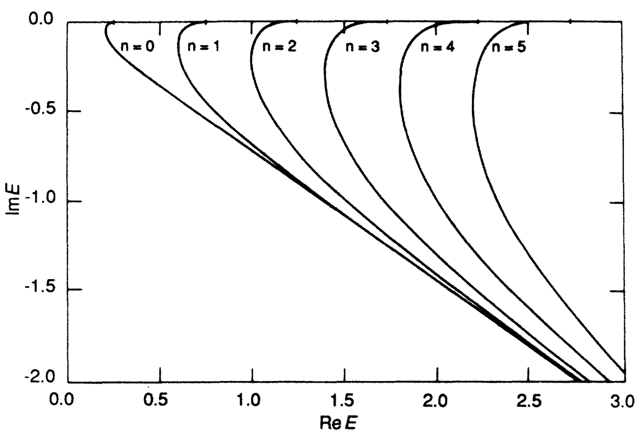

FIG. 1. Plot of the first six resonance eigenvalues of the cubic anharmonic oscillator—with $m=1$, $\hbar=1$, $k=\frac{1}{4}$—in the complex plane as the perturbation strength g increases from 0 towards ∞.

ed matrices defined in Eq. (36). Consequently, it is necessary to set up a criterion to choose optimum (in a certain sense) parameters $\mathrm{Re}\theta_0$, $\mathrm{Im}\theta_0$. A convenient criterion follows from the stationary condition[13] with respect to θ, which, with Eq. (32) for the infinitesimal generator, can be written

$$\langle \Psi(\theta^*),[H(\theta),A]\Psi(\theta)\rangle=0\ , \tag{37}$$

and which, for Eq. (33), takes the form

$$e^{-2\theta}\langle \Psi(\theta^*),\tfrac{1}{2}p^2\Psi(\theta)\rangle=e^{2\theta}\langle \Psi(\theta^*),\tfrac{1}{2}kx^2\Psi(\theta)\rangle + \tfrac{3}{2}e^{3\theta}\langle \Psi(\theta^*),gx^3\Psi(\theta)\rangle\ . \tag{38}$$

Equation (38) can be viewed as a complex generalization of the virial theorem. The parameters $\mathrm{Re}\theta_0$, $\mathrm{Im}\theta_0$ have been chosen in each case to insure numerical satisfaction of Eq. (38).

Figure 1 shows the behavior of the resonances coming from the six lowest bound states of the harmonic oscillator of force constant $k=\frac{1}{4}$ (to make easier the comparison with previous results[14]), and Table I shows some numerical values for the resonances coming from the two lowest bound states.

The inverse vector iteration algorithm[15] (with explicit error bound estimates and a generalization of Rayleigh's quotient to speed up convergence) has been used to calculate selected eigenvalues of the complex symmetric matrices (36). The numerical results given in this section have been obtained with an exhaustive analysis of convergence, including calculations with nonoptimal parameters. Numerical evidence is that all the figures shown are exact. As was to be expected, narrow resonances are well represented with a small number of basis functions, the limiting factor on the precision being the fact that $\Gamma/2 \ll E_r$. Broader resonances require more basis functions, but even with nonoptimal parameters, $N=100$ is sufficient to achieve the convergence to the number of figures shown in the tables.

Since the RSPT series is Borel summable with analytic continuation, one can use the Borel-Padé method to get resonance eigenvalues numerically. For comparison, Table II shows some results for the numerical Borel-Padé sum of the ground state. The details are as follows. From the perturbation series, the Borel transformed series is generated by

$$B_0(g)=\sum_{N=0}^{\infty} E_0^{(N)}\frac{g^N}{N!} \tag{39}$$

and resummed numerically

TABLE I. Resonances coming from the two lowest eigenvalues of the harmonic oscillator of force constant $k=\frac{1}{4}$, as a function of the coupling constant g, calculated by the variational method with complex rotation.

	Ground state, $n=0$		First excited state, $n=1$	
g	$\mathrm{Re}E(g)$	$-\mathrm{Im}E(g)$	$\mathrm{Re}E(g)$	$-\mathrm{Im}E(g)$
0.015	0.244 597 357 025 2	0.000 000 027 685 6	0.711 461 228 615 7	0.000 020 470 810 6
0.020	0.239 396 653 193 9	0.000 062 728 114 3	0.661 830 135 813 8	0.011 634 444 958 2
0.025	0.230 644 774 104 2	0.001 783 751 534 5	0.615 671 596 186 4	0.069 793 563 306 5
0.030	0.220 211 295 733 9	0.008 782 012 944 0	0.603 742 619 952 7	0.139 292 387 331 3
0.035	0.212 365 637 906 4	0.020 317 481 587 1	0.611 114 517 402 0	0.200 340 877 051 2
0.040	0.208 164 464 309 3	0.033 488 394 680 9	0.626 959 480 069 1	0.251 851 033 963 4
0.045	0.206 880 979 819 5	0.046 579 252 284 5	0.646 470 774 926 8	0.295 774 699 643 1
0.050	0.207 625 482 618 3	0.058 912 651 268 2	0.667 492 314 119 0	0.333 897 961 469 3
0.060	0.212 708 228 171 7	0.080 743 198 901 4	0.710 441 950 070 7	0.397 663 013 604 0
0.070	0.220 212 281 173 3	0.099 135 819 821 2	0.752 273 886 293 1	0.449 943 177 434 3
0.080	0.228 693 719 090 2	0.114 821 547 722 0	0.792 103 158 003 3	0.494 477 158 760 9
0.090	0.237 488 353 921 4	0.128 434 957 833 3	0.829 807 017 936 0	0.533 477 267 246 9
0.100	0.246 281 518 695 5	0.140 449 526 600 8	0.865 497 606 347 5	0.568 340 948 119 4
0.500	0.466 391 109 824 3	0.333 997 289 372 0	1.659 631 602 678 9	1.197 954 615 648 8
1.000	0.616 476 811 580 1	0.445 852 050 920 0	2.192 077 856 063 4	1.589 299 601 446 3
5.000	1.174 745 089 401 7	0.853 216 340 477 0	4.175 109 029 887 6	3.032 921 130 854 5
10.000	1.550 185 234 284 4	1.126 151 807 149 7	5.509 259 579 612 6	4.002 506 209 192 3
100.000	3.894 013 382 829 2	2.829 158 578 203 9	13.838 843 371 588 6	10.054 495 357 915 5

TABLE II. Resonance coming from the lowest eigenvalue of the harmonic oscillator of force constant $k=\frac{1}{4}$, as a function of the coupling constant g, calculated via Borel-Padé sum with a [50/50] Padé approximant.

g	$\text{Re}E(g)$	$-\text{Im}E(g)$
0.015	0.244 597 357 025 2	0.000 000 027 686 6
0.020	0.239 396 653	0.000 062 728
0.025	0.230 644 8	0.001 783 8
0.030	0.220 211	0.008 782

$$E_0(g)=\alpha\int_0^\infty e^{-\alpha t}B_0(\alpha t g)dt$$
$$\approx\alpha\int_0^\infty e^{-\alpha t}P^{[M/M]}(\alpha t g)dt\ . \quad (40)$$

The choice of the parameter α (that is, the path of integration in the complex plane) is such that the Padé approximants seem to have no poles along it. Slight variations do not have substantial effect in the precision, unless α approaches the real axis, where the Padé approximants do have poles. It was convenient to take α halfway between the real and imaginary axis, $\alpha=i^{1/2}[\arg(\alpha)=\pi/4.]$ The integration has been carried out numerically by two independent methods (Gauss-Laguerre quadrature and Gauss-Legendre quadrature with multiple finite intervals). Although much faster than the complex dilation calculations, precision is rapidly lost as the coupling constant increases.

V. CONCLUSIONS

The cubic anharmonic oscillator is a prototypical system exhibiting resonances. By means of JWKB techniques in the complex plane and numerical computations, a complete picture of the behavior of the resonances in the whole range of coupling-constant values has been presented (Fig. 1).

In the limit of a small coupling constant, the quasisemiclassical method[9] allows one to construct an explicit asymptotic expansion for the imaginary part of the resonances. This expansion turns out to be exponentially small with respect to the RSPT series, a fact which can be intuitively understood in terms of tunneling through the potential barrier.

The relation between this asymptotic expansion and the familiar RSPT series can be viewed at least in two ways. On one hand, the RSPT is Borel summable to give both the real and imaginary parts of the resonances. (Although of limited practical applicability, the Borel sum can be carried out numerically.) On the other hand, the asymptotic expansion for the imaginary part of the resonances determines, via a dispersion relation, the large-N asymptotic behavior of the RSPT energy coefficients.

The JWKB method also allows the determination of the large coupling-constant behavior, providing insight into a previous rigorous result by Sibuya. In fact, Sibuya's derivation shows that these resonances remain in the pure cubic case $V=gx^3$, where there is no potential barrier on the real axis as there is when $V=kx^2/2+gx^3$.

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[2]The minimal operator generated by the action of (1) on the space of all infinitely differentiable functions of compact support admits infinitely many self-adjoint extensions (Ref. 3), and there is no physical criterion to single out one of them. This is the quantum analogue of the fact that a classical particle initially moving in $(-\infty,-k/3g)$ takes a finite time to reach $x=-\infty$. These situations are called incomplete (Ref. 4). Although, in general, neither of the implications classically incomplete$\Longleftrightarrow$quantum incomplete is true, for the cubic oscillator the problem is incomplete in both senses.

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