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BRIEF COMMUNICATION

Infinite square well with a sinusoidal bottom: a candidate for the Klauder phenomenon?

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Abstract In contrast to a recent observation, we notice that a particle in a box with any cosine bottom does not show up the Klauder phenomenon when the perturbation is gradually reduced to zero. Both perturbative and variational approaches have been pursued. The case of a harmonic oscillator perturbed by a similar potential is additionally studied. No peculiarity is observed anywhere in this case too. Possible reasons behind the phenomenon are sought to rationalize our findings.

Keywords Perturbation theory · Klauder phenomenon · Sinusoidal potential

1 Introduction

Recently [1], in course of extending a class of exactly solvable one-dimensional systems, attention has been focused on the energy spectra of a particle in a square well potential with various sinusoidal bottoms as examples. Interestingly, pursuit of the above study has revealed [1,2] that, under certain circumstances, usual results for energy of the flat bottom case do not follow even if one allows the sinusoidal potentials to vanish. Instead, states arrange themselves from some new lowest-energy eigenvalues. This is referred to as a type of Klauder phenomenon [3–6] (KP) which states that some vestigial effects may be retained by quantum states for specific perturbations even when the latter tend to vanish.

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To be specific, here the problem is concerned with a box potential in $(0, L)$ whose flat bottom at zero potential is modified by introducing any additional potential of the form $\lambda \cos(k\pi x/L)$, with $k = 1, 2, 3, \ldots$ It has been claimed [1] that, *except* for $k = 1$, results for the perturbed ground state energy do not reduce to that of the parent box potential in the limit $\lambda \to 0$. Always, one observes positive shifts in energies of the states. In particular, the unperturbed box energies E_n $(n = 1, 2, \ldots)$ change to $(k\pi/L)^2 E_n$. This feature is referred to as a kind of the KP.

An independent analysis of the above problem is imperative. This is because, if the observations [1] are correct, it remains to be explained that the KP is indeed not restricted to potentials that are singular at a finite point of space, as is commonly believed [6]. Needless to mention, the cosine perturbation is bounded.

2 Perturbative analysis

We first apply the standard Rayleigh-Schrdinger perturbation theory [7–9] (RSPT) to the above problem at two different values of k. The choices would suffice to establish our contention. RSPT does not encounter any difficulty for any of the above selection, and we obtain the following results for the ground state energy at the lowest orders of perturbation, choosing $m = 1/2$ and $\hbar = 1$:

$$\begin{aligned} E_1\,(k=1,\ \lambda) &= \left(\frac{\pi}{L}\right)^2 - \lambda^2 \frac{L^2}{12\pi^2} + \boldsymbol{O}\left(\lambda^4\right) \\ E_1\,(k=2,\ \lambda) &= \left(\frac{\pi}{L}\right)^2 - \frac{\lambda}{2} - \lambda^2 \frac{L^2}{32\pi^2} + \lambda^3 \frac{L^4}{512\pi^4} + \boldsymbol{O}\left(\lambda^4\right) \end{aligned} \tag{1}$$

These results do reveal that the ground state energy of the box is regained under the limit $\lambda \to 0$ for each of the cases considered. There is no shift in the lowest energy for $k = 2$. Moreover, the potential for $k = 2$ is symmetric about $L/2$ and hence has a non-vanishing first order correction that the $k = 1$ perturbation does not have.

Perturbation series for the wave functions again bring to light the regular character in the $\lambda \to 0$ limit, as found above. The parent box states show up in both the cases under scrutiny. This is evident from the expansions that we have worked out,

$$\begin{aligned} \Psi_1\,(k=1,\ \lambda) &= \Phi_1 - \lambda \frac{L^2}{6\pi^2}\Phi_2 + \lambda^2 \frac{L^4}{96\pi^4}\Phi_3 + \boldsymbol{O}\left(\lambda^3\right) \\ \Psi_1\,(k=2,\ \lambda) &= \Phi_1 - \lambda \frac{L^2}{16\pi^2}\Phi_3 + \lambda^2 \frac{L^4}{256\pi^4}\left[\Phi_3 + \frac{1}{3}\Phi_5\right] + \boldsymbol{O}\left(\lambda^3\right) \end{aligned} \tag{2}$$

where states Φ_j refer to the normalized parent box states, given by

$$\Phi_j = \sqrt{\frac{2}{L}} \sin \frac{j\pi x}{L}. \tag{3}$$

The role of symmetry is once again notable. The state retains its symmetry around $L/2$ only for the $k = 2$ case and this is clear from the second equation in (2) that

shows mixing of *specific* states, in contrast to the situation for $k = 1$. Thus, RSPT yields series for wave functions with no special trait for $k = 2$ except for symmetry. No KP is apparent anywhere. We do not also find any reason for the appearance of an extra node in the ground state at $k = 2$ (see Fig. 4 of Ref. 1).

It may be of interest to also know how the ground state energy depends on the perturbation for large k. Actually, the large-k limit is particularly significant because we expect on physical ground that too many oscillations of a cosine function over a finite domain should average out to zero. Hence, one is inclined to think that the correction would be smaller with rising k. Indeed, proceeding via a perturbative route, one obtains the leading correction to the ground state energy as

$$-\lambda^2 \frac{L^2}{2\pi^2\left(k^2-4\right)} \tag{4}$$

for any $k \geq 3$. This explicitly shows how quickly the correction becomes insignificant at large k. No question of any huge shift of the lowest energy arises.

3 Variational analysis

To further substantiate our contention, one may like to adopt a variational analysis following the Rayleigh-Ritz principle. This is an altogether independent approach whereby one can check how the different ground-state energies of the perturbed problem behave as the coupling constant is gradually reduced to zero. We employ the box bases [10] and follow a linear variational strategy that is known to furnish quite reliable results. Figure 1 shows how the near-exact lowest energies behave at a sample value of $L = 1$. Here, for convenience, we have used a logarithmic scale for the abscissa. Note that they reach the same unperturbed value (π^2) quite smoothly in both the cases under scrutiny. This corroborates our findings on the basis of RSPT. Thus, no special status can be ascribed to the case $k = 1$.

The above variational procedure can be pushed to gain further advantage. Had there been really a KP of the sort argued, one expects that the perturbation $\lambda\cos(k\pi x)$ would increase the ground state energy by a factor of $(k\pi)^2$ and this factor rises sharply with k. On the other hand, as stated before, the potential $\lambda\cos(k\pi x)$, for any high value of k, would show only rapid oscillations about zero, the flat bottom of the box. Effectively, then, this should render the ground state energy virtually unchanged. Indeed, such a situation is observed in our calculations too. Table 1 shows the behavior of the ground state energy for two very different values of the coupling constant. One really notes that the parent box energy is virtually regained at large k *even* when $\lambda = 1$. Smaller k values yield the limiting result at smaller λ, as expected. Therefore, our contention that there should be no shift of the parent ground energy is not only true in the $\lambda \to 0$ limit for any k, it is true even at a finite λ for large k as well! Since variational results always provide upper bounds to true energies, and the concerned Hamiltonians are bounded from below, one can confide on these results.

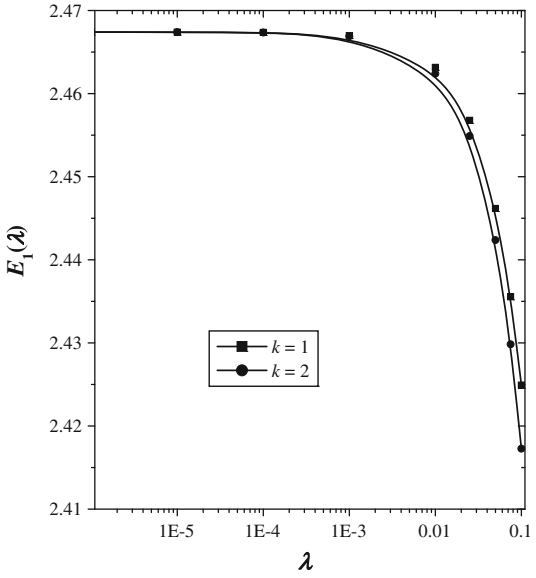

Fig. 1 Plots of near-exact energies for ground states in potentials $\lambda\cos(k\pi x/L)$ at $L = 1$ within a square well in (0, 1). The bare box result is approached in both the cases as $\lambda \to 0$

Table 1 Behavior of the ground state energy for the perturbation $\lambda\cos(k\pi x)$ on a particle in a box in (0, 1) at large k

k	$\lambda = 1.0$	$\lambda = 0.0001$
10	9.869077	9.869604401
20	9.869476	9.869604401
40	9.869572	9.869604401
60	9.869590	9.869604401
80	9.869596	9.869604401
100	9.869602	9.869604401

4 Harmonic oscillator with a cosine perturbation

Let us now briefly look at the problem of a harmonic oscillator perturbed by a similar cosine potential $\lambda\cos(k\pi x)$. We expect that results would not differ much from the box case under any situation, be it $k = 1$ or $k \neq 1$. Indeed, the perturbed ground state energy of the Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 + \lambda\cos(k\pi x) \tag{5}$$

shows the following variation with k as we proceed via RSPT:

$$E_0 = 1 + \lambda\exp\left[-k^2\pi^2/4\right] + \lambda^2\exp\left[-k^2\pi^2/2\right]\varepsilon(k) + O\left(\lambda^3\right). \tag{6}$$

Result (6) is true for any k, and here the sum-over-states representation of the second order energy correction term fortunately admits a closed form description. Thus, the

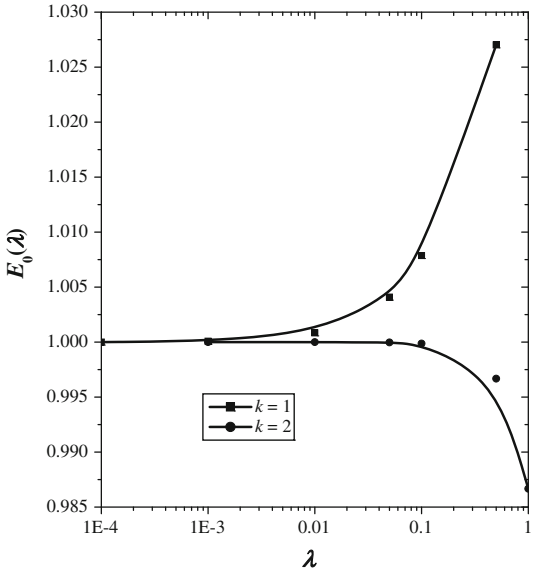

Fig. 2 Plots of near-exact energies for ground states in potentials $x^2 + \lambda\cos(k\pi x/L)$. The bare harmonic oscillator result is approached in both the cases as $\lambda \to 0$

factor $\varepsilon(k)$ in (6) is expressible as

$$\varepsilon(k) = \frac{1}{2}\left[\gamma + \ln\frac{k^2\pi^2}{2} - Chi\left(\frac{k^2\pi^2}{2}\right)\right], \tag{7}$$

γ being the Euler constant. Using the definition of $Chi(x)$

$$Chi(x) = \gamma + \ln x + \int_0^x \frac{\cosh t - 1}{t} dt \tag{8}$$

one can also express $\varepsilon(k)$ as a series:

$$\varepsilon(k) = -\frac{1}{2}\sum_{j=1}^{\infty} \frac{x^{2j}}{(2j)!\,(2j)}, \quad x = k^2\pi^2/2. \tag{9}$$

The important point here is that the second order energy is exactly summable. One can also see from (6) and (7) how rapidly the correction terms decay with k, as we expected.

We have noted in Fig. 1 how lowest energies of box systems under the potential $\lambda\cos(k\pi x)$ at the two chosen k-values behave with λ. The situation with the harmonic oscillator case is similar. By following the same variational procedure as adopted earlier, we have obtained Fig. 2 that shows the change of ground energy for the total potential $x^2 + \lambda\cos(k\pi x)$ as λ is varied. A smooth passage to the unperturbed energy is quite apparent in both the chosen cases. No shift arises here either.

5 Notes on the Klauder phenomenon

It now remains to explain why such a sinusoidal perturbation problem is an unlikely candidate to show up the KP. This is most directly seen by casting the stationary Schrodinger equation for the perturbed problem in the Riccati form that looks as

$$\chi_n^2 + \chi_n' + E_n - V = 0 \tag{10}$$

where $\chi_n = \Psi_n'/\Psi_n$. Consider now a potential of the form

$$V = x^2 + \lambda/x^\beta,\ \beta > 2, \tag{11}$$

that has attracted considerable attention [6,11–13] in this context. The perturbing potential here is singular at the origin. A look at the small-x behavior of χ_n on the basis of (10) yields

$$\chi_n = \frac{\sqrt{\lambda}}{x^{\beta/2}}. \tag{12}$$

This gives

$$\lim_{x\to 0} \Psi_n(\lambda) = \exp\left[\frac{2\sqrt{\lambda}}{2-\beta} x^{1-\beta/2}\right]. \tag{13}$$

For the unperturbed problem, the wave function goes to zero as x, but (13) tends to vanish much more steeply. Moreover, in the $\lambda \to 0$ limit, the signature of perturbation is more enduring in the wave function, because of the $\sqrt{\lambda}$ dependence in (13), compared to the potential (11). A similar analysis is true of the H atom problem perturbed by a similar potential, as may be easily checked. In such cases, there is a qualitative change in the nature of $\Psi_n(\lambda)$in the small-x region relative to the unperturbed wave function. Thus we notice the major aspects of the KP. First, the domains of the perturbed and unperturbed Hamiltonians (H and H_0) are different. Hence, one experiences that

$$\lim_{\lambda\to 0} H(\lambda) \neq H_0. \tag{14}$$

This additionally means, the perturbed spectra do not coincide with the unperturbed one even in the limit of zero coupling strength. Our present problem has surfaced precisely in such a context. Secondly, the point singularity in the perturbing potential is essential to validate (14). If the unperturbed and perturbing potentials are singular at the same point, the latter has to be more singular to show up KP. This is a necessary condition, but not sufficient. For example, The H atom problem perturbed by a $1/r^2$ potential does not reveal any sort of KP. Thirdly, while KP ensures sustained memory effects, the converse is not true in general. Indeed, perturbing potentials that are more singular near the boundaries show a similar feature in the large-x regime. For example,

with anharmonic oscillators of the form

$$V = x^2 + \lambda x^{2N} \quad [N = 2,\ 3, \ldots] \tag{15}$$

one obtains from (10)

$$\lim_{x\to\infty} \chi_n = -\sqrt{\lambda} x^N \tag{16}$$

and hence

$$\lim_{x\to\infty} \Psi_n(\lambda) = \exp\left[-\frac{\sqrt{\lambda}}{N+1} x^{N+1}\right]. \tag{17}$$

While any unperturbed oscillator state decays as $\exp\left[-x^2\right]$, (17) shows that there is a qualitative change now even when $\lambda \to 0$. Also, $\Psi_n(\lambda)$ has a softer λ-dependence than V in (15).

6 Final remarks

A few more points need to be stressed. (i) The KP is usually discussed [6,11–13] in the context of perturbing potentials like (11). This is because, here one often encounters non-Taylor expansions [14] for energy. The reason can be traced back to the λ-dependence of the dominant integrals in the Rayleigh quotient where (13) plays a decisive role. More complicated are supersingular perturbations ($\beta \geq 3$) for which even the first order RSPT corrections to energy become infinite. Anharmonic oscillators of the form (15) induce insignificant contribution to the energy integrals from (17) as this region is far off from the potential minima. Therefore, these oscillators lack the peculiarity for which the KP is mainly fascinating, viz. energy shifts [equivalently, (14)] and the emergence of perturbation series with bizarre λ-dependence [6]. (ii) The memory effects of some singular perturbations last longer in the wave functions than in the potentials primarily because of (10). One sees clearly that V is directly linked with χ_n^2, and not Ψ_n. Hence, status of the coupling constant is different in the wave function and in the Hamiltonian. This is precisely responsible for sustained memory. In this respect, potentials (15) do show some promise in spite of the fact that they do not satisfy the Klauder condition. (iii) Singular potentials like (11) pose considerable challenge to variational calculations [15–18] as well owing to the peculiar form (13) of the true wave function near the origin. The cosine perturbation under investigation here does not possess any singularity. Hence, both the perturbative and variational calculations are hassle-free. Therefore, KP does not show up here. (iv) Various sum rules are nicely obtained from studies in RSPT [19,20]. For the Hamiltonian (5), our results (6) and (7) do reveal the emergence of a class of new sum rules for the second order energy that is valid for arbitrary k.

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