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On the linear dispersion–linear potential quantum oscillator

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ABSTRACT

We solve the bi-linear quantum oscillator $H = v|p| + F|x|$ both quasi-classically and numerically.

1. Introduction

With the quantum theory, as it was called at the time, nearing its first centennial anniversary, it is a rare opportunity to study a one-dimensional ideal oscillator which has not been solved long ago. The motion of a (non-relativistic) quantum particle with a linear dispersion, $\epsilon_p = v \cdot |p|$, where $p = \hbar k$ is the momentum and v is a parameter, in a linearly confining potential $V(x) = F \cdot |x|$, where x is the position and the constant force F again a parameter, however, appears to provide an example. While the problem may look trivial at first, it is not. The usual method of quantization by replacing either $p \to -i\hbar\frac{\partial}{\partial x}$ or $x \to i\hbar\frac{\partial}{\partial p}$ cannot be applied directly, as one cannot sensibly define the absolute value of a differential operator.

The problem is not just of academic interest, but even of relevance to a recent experiment [1,2]. Spinons, the fractionally quantized and elementary excitations in antiferromagnetic spin chains, are well known to disperse linearly at low energies, with v proportional to the antiferromagnetic exchange constant J along the chains [3]. Spinons carry the spin of an electron but no charge. Since the anti-particle for a spinon is just another spinon with its spin reversed, the spectrum has only a positive energy branch. As one couples two chains antiferromagnetically [4], the coupling $J_\perp$ will induce a linear

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confinement potential between pairs of spinons, as the rungs between two spinons become effectively decorrelated [5,6]. To a very first approximation, the energy gap in the spin ladder is hence given by the ground state energy of the bi-linear oscillator

$$H = v|p| + F|x|, \tag{1}$$

which we study in this article. The ground state is symmetric under one-dimensional parity $x \to -x$ and corresponds to a spinon pair in the triplet channel, while the first excited state is antisymmetric under $x \to -x$ and corresponds to the lowest singlet excitation in the spin ladder. It the context of this problem, it is hence desirable to know what the lowest eigenvalues of Eq. (1) are. From dimensional considerations, it is immediately clear that they must scale like $\sqrt{\hbar v F}$.

2. Quasi-classical approach

Even though the usual method of quantization cannot be applied directly, the problem can still be approached quasi-classically. Applying the Bohr–Sommerfeld quantization condition [7]

$$\frac{1}{2\pi\hbar}\oint p dx = n + \frac{1}{2}, \tag{2}$$

where the integration extends over the entire classical orbit, results with $p(x) = \frac{E_n - F|x|}{v}$ in

$$\frac{1}{2\pi\hbar} 4 \int_0^{E_n/F} \frac{E_n - Fx}{v} dx = n + \frac{1}{2}. \tag{3}$$

Carrying out the integration yields

$$E_n = \sqrt{\pi\left(n + \frac{1}{2}\right)} \cdot \sqrt{\hbar v F}. \tag{4}$$

We expect this to constitute a reasonable approximation for the higher energy levels, but probably not for the low lying ones. Indeed, this is what we will find as we solve the problem numerically below.

3. Mathematical formulation

Before proceeding with the numerical solution, let us rewrite the eigenvalue equation $H\psi(x) = E\psi(x)$ as a differential (and integral) equation in position space. For convenience, we consider the dimensionless Hamiltonian

$$H = |k| + |x|, \tag{5}$$

which is obtained from Eq. (1) by rescaling

$$\frac{H}{\sqrt{\hbar v F}} \to H, \quad \sqrt{\frac{\hbar v}{F}} k \to k, \ \text{and} \ \sqrt{\frac{F}{\hbar v}} x \to x. \tag{6}$$

Let us denote the eigenvalues of Eq. (5) by λ and the eigenfunctions by $\phi(x)$. With

$$\tilde{\phi}(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(x) e^{-ikx} dx, \tag{7}$$

$$\phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{\phi}(k) e^{ikx} dk, \tag{8}$$

we may write

$$
\begin{aligned}
|k|\phi(x) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} k\ \mathrm{sign}(k)\tilde{\phi}(k)e^{ikx}dk \\
&= -i\frac{\partial}{\partial x}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \mathrm{sign}(k)\tilde{\phi}(k)e^{ikx}dk \\
&= -i\frac{\partial}{\partial x}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \tilde{s}(x-x')\phi(x')dx',
\end{aligned}
\tag{9}
$$

where

$$
\mathrm{sign}(k) = \begin{cases} +1 & k\geq 0 \\ -1 & k<0 \end{cases}
$$

is the sign function and

$$
\begin{aligned}
\tilde{s}(x) &= \frac{1}{\sqrt{2\pi}}\lim_{\epsilon\to 0}\int_{-\infty}^{\infty} \mathrm{sign}(k)e^{-\epsilon|k|}e^{ikx}dk \\
&= \frac{2i}{\sqrt{2\pi}}\lim_{\epsilon\to 0}\frac{x}{x^2+\epsilon^2} = \frac{2i}{\sqrt{2\pi}}\mathcal{P}\frac{1}{x},
\end{aligned}
\tag{10}
$$

where $\mathcal{P}$ denotes the principal part, is the Fourier transform thereof. The eigenfunctions $\phi(x)$ with eigenvalues λ of Eq. (5) are hence the solutions of

$$
\frac{1}{\pi}\frac{\partial}{\partial x}\mathcal{P}\int_{-\infty}^{\infty}\frac{\phi(x')}{x-x'}dx' + |x|\phi(x) = \lambda\phi(x)
\tag{11}
$$

While Eq. (11) provides a clear mathematical formulation of the problem, we are not aware of any method to solve it analytically, nor consider it a viable starting point for numerical work.

4. Numerical solution

To solve Eq. (5) numerically, we exactly diagonalize a finite Hamiltonian matrix we obtain through discretization of position space with a suitably chosen cutoff.

Let this discrete Hilbert space consist of N sites, with the positions

$$
x_i = a\left(i-\frac{N+1}{2}\right)
\tag{12}
$$

where $i=1, 2, \ldots N$ and a is the lattice constant. The cutoff $|x_c|=Na/2$ in real space implies a cutoff

$$
\lambda_c = \frac{Na}{2}
\tag{13}
$$

for the potential energy in Eq. (5), which must be chosen significantly larger than the largest eigenvalue λ_n we wish to evaluate reliably. (From Eq. (4), we expect λ_n to be of order $\sqrt{\pi\left(n+\frac{1}{2}\right)}$.) On the other hand, the classically allowed part of the Hilbert space will contain only of the order of N/λ_c sites for the ground state, which implies that we must further require $\lambda_c \ll N$.

The lattice provides us simultaneously with a cutoff in momentum space, $-\pi\leq ak\leq\pi$. We may hence expand $|k|$ in a Fourier series,

$$
|ak| = \frac{b_0}{2} + \sum_{m=1}^{\infty} b_m\cos(mak)
\tag{14}
$$

with

$$b_m = \frac{1}{\pi}\int_{-\pi}^{\pi} dk|k|\cos(mk) = \begin{cases} \pi & m=0 \\ -\frac{4}{\pi}\frac{1}{m^2} & m\,\text{odd} \\ 0 & \text{otherwise} \end{cases}, \tag{15}$$

as one may easily verify through integration by parts. We proceed by writing Eq. (5) in second quantized notation,

$$\begin{aligned} H &= \sum_k |k|c_k^\dagger c_k + \sum_i |x_i|c_i^\dagger c_i \\ &= \frac{1}{a}\sum_k |ak|c_k^\dagger c_k + a\sum_i \left|i - \frac{N+1}{2}\right| c_i^\dagger c_i \end{aligned} \tag{16}$$

where

$$c_k^\dagger = \frac{1}{\sqrt{N}}\sum_i e^{ikx_i}c_i^\dagger, \quad c_i^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{-ikx_i}c_k^\dagger. \tag{17}$$

Since

$$\sum_k \cos(mak)c_k^\dagger c_k = \frac{1}{2}\sum_i \left(c_i^\dagger c_{i+m} + h.c.\right), \tag{18}$$

we obtain

$$H = \sum_{i,j=1}^{N} c_i^\dagger h_{ij} c_j \tag{19}$$

with

$$h_{ij} = \begin{cases} \frac{N}{2\lambda_c}\frac{\pi}{2} + \frac{2\lambda_c}{N}\left|i - \frac{N+1}{2}\right| & i=j \\ -\frac{N}{2\lambda_c}\frac{2}{\pi}\frac{1}{(i-j)^2} & i-j\,\text{odd} \\ 0 & \text{otherwise} \end{cases}, \tag{20}$$

where we have substituted $\frac{2\lambda_c}{N}$ for a.

Numerical diagonalization of h_{ij} yields the eigenvalues λ_n and eigenfunctions $\phi_n(x_i)$ of Eq. (5), and hence the eigenvalues and eigenfunctions

$$E_n = \lambda_n\sqrt{\hbar v F}, \quad \psi_n(x) = \phi_n\left(\sqrt{\frac{F}{\hbar v}}x\right) \tag{21}$$

of Eq. (1). The results for $N = 20{,}001$, $\lambda_c = 20$ are listed in Table 1 and Figs. 1 and 2. (We have chosen an odd number for N, because this means that the position $x = 0$, where the potential $|x|$ is not differentiable, coincides with a lattice point. Including this point improves the convergence of the eigenvalues and functions for n even.) From Table 1, we see that the quasi-classically obtained eigenvalues converge towards the numerically obtained values as n is increased.

The eigenfunctions obtained numerically can be approximated by

$$\phi_n(x) = x^n\exp\left(-a_n\sqrt{x^2 + b_n^2} + c_n\right) \tag{22}$$

Table 1
Eigenvalues λ_n for $n = 0, \ldots, 19$ obtained by exact diagonalization of Eq. (20) for $N = 20{,}001$, $\lambda_c = 20$. From the scaling behavior with N and comparisons of different values for λ_c, we estimate the error due to the finite size to be less than ± 0.00002 for n even and ± 0.00001 for n odd. For comparison, we also list the quasi-classical values (Eq. (4)).

m	λ_{2m}	λ_{2m+1}	λ_{2m}	λ_{2m+1}
	Numerically		Quasi-classically	
0	1.10408	2.23229	1.2533	2.1708
1	2.77281	3.33002	2.8025	3.3160
2	3.75118	4.16416	3.7599	4.1568
3	4.51300	4.85855	4.5189	4.8541
4	5.16402	5.46623	5.1675	5.4631
5	5.74065	6.01303	5.7434	6.0107
6	6.26457	6.51426	6.2666	6.5124
7	6.74763	6.97965	6.7493	6.9782
8	7.19841	7.41595	7.1997	7.4147
9	7.62246	7.82800	7.6236	7.8269

for $n = 0$, 1 and by

$$\phi_n(x) = x^{n-2}\left(d_n^2 - x^2\right) exp\left(-a_n\sqrt{x^2 + b_n^2} + c_n\right) \tag{23}$$

for $n = 2, 3$, with parameters a_n, b_n, c_n, and d_n listed in Table 2. Comparisons of these fits to the numerically obtained eigenfunctions are shown in Fig. 3. The fits are not as good an approximation as Fig. 3 may suggest, however, as they fall off as $\exp(-a|x|)$ while the true eigenfunctions $\phi_n(x)$ fall off as $1/x^3$ for n even and as $1/x^4$ for n odd as $x \to \infty$.

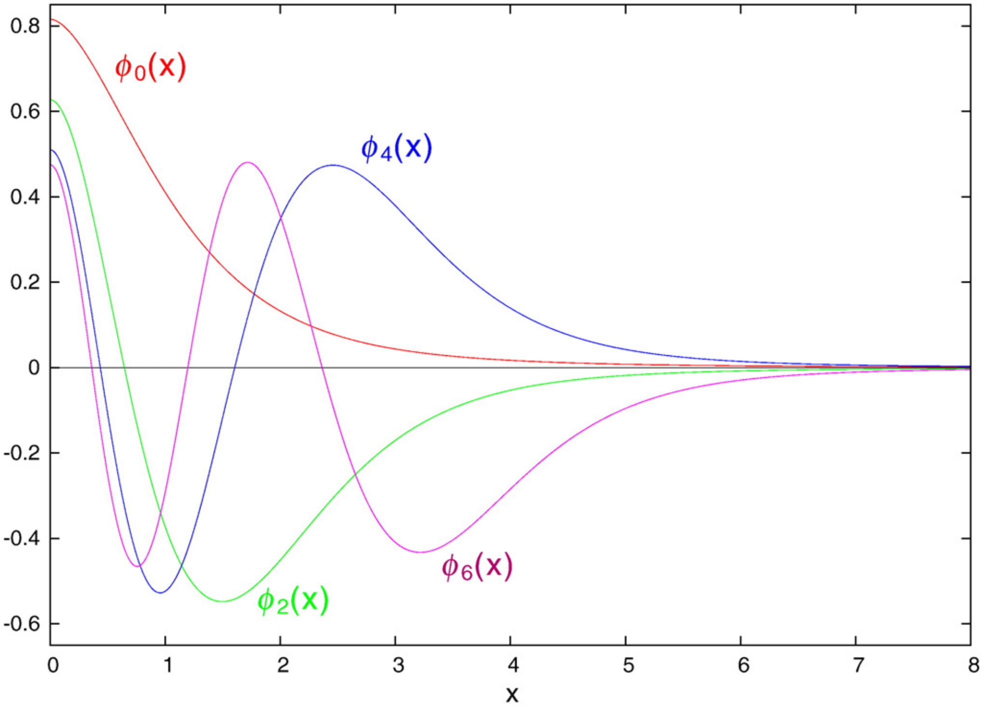

Fig. 1. The first four symmetric eigenfunctions $\phi_n(-x) = \phi_n(x)$ for n even obtained numerically for $N = 20{,}001$, $\lambda_c = 20$.

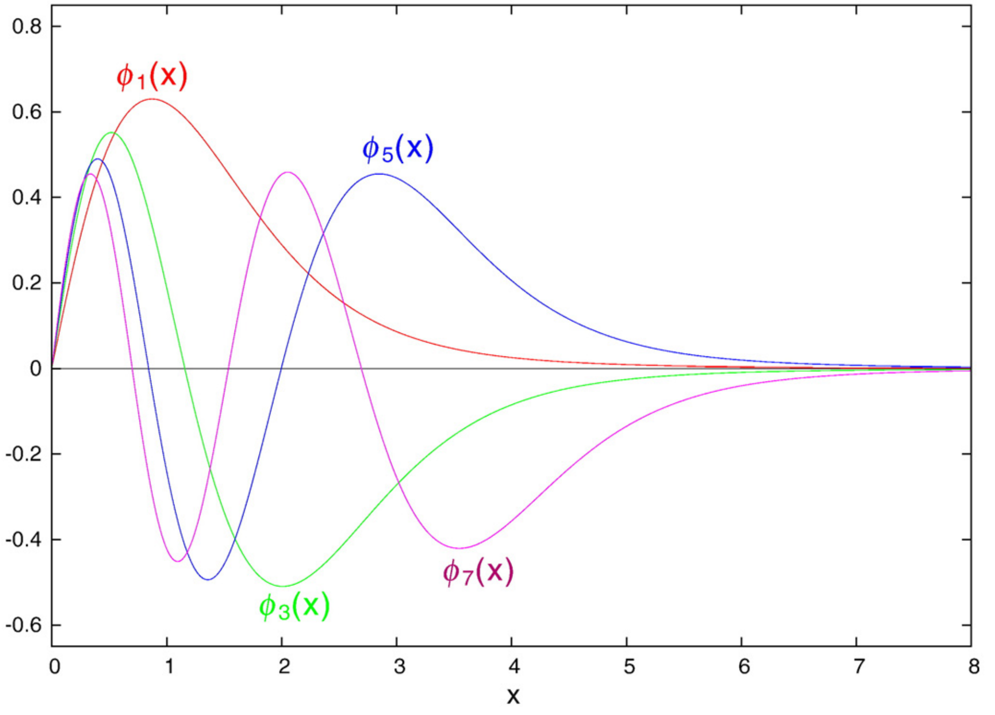

Fig. 2. The first four antisymmetric eigenfunctions $\phi_n(-x) = -\phi_n(x)$ for n odd obtained numerically for $N = 20{,}001$, $\lambda_c = 20$.

This asymptotic behavior of the eigenfunctions can be understood physically through second order perturbation theory. If we consider a small region around a point $x \gg \lambda$ (*i.e.*, very far away from the classically allowed region for the eigenstate with energy λ), the amplitude there will be governed by scattering into this region from the classically allowed region, which contains almost the entire amplitude of the state. From Eq. (20), this scattering is proportional to

$$\int_{-\lambda_n-\lambda_t}^{\lambda_n+\lambda_t} \frac{\phi_n(x')}{(x-x')^2}\,dx' \propto \begin{cases} \dfrac{1}{x^2} & n \text{ even} \\ \dfrac{1}{x^3} & n \text{ odd} \end{cases}, \tag{24}$$

where λ_t is a cutoff to ensure that we include the tail immediately surrounding the classically allowed region in the integral (from Figs. 1 and 2, we see that $\lambda_t = 3$ would be a reasonable choice). With the potential energy in the region we consider given by $|x|$, the amplitude for finding the particle there will be proportional to $1/x^3$ for n even and as $1/x^4$ for n odd.

Table 2
Parameters obtained numerically from fitting Eqs. (22) and (23) to the functions $\phi_n(x)$ obtained by exact diagonalization of Eq. (20) for $N = 20{,}001$, $\lambda_c = 20$.

n	a_n	b_n	c_n	d_n
k	1.1849	0.57196	0.4681	
1	1.7443	0.96843	1.9494	
2	1.9517	0.94194	2.2398	0.64431
3	2.2842	1.17617	2.9428	1.15453

The numerical work reported here indicates that, within the limits of accuracy, the solutions are differentiable at $x = 0$, *i.e.*, the expansion of $\phi_n(x)$ around $x = 0$ does not contain a term proportional to $|x|$ for n even or $x|x|$ for n odd. Unfortunately, we have not been able to reach a conclusion regarding higher terms, and cannot tell whether there are terms proportional to $x^2|x|$ for n even or $x^3|x|$ for n odd.

5. Further considerations

It would be highly desirable to identify the exact eigenvalues and functions of Eq. (5). Unfortunately, we have as of yet not even succeeded in obtaining those for the ground state. A few thoughts on this problem, however, are possibly worth mentioning.

5.1. Fourier symmetry

As the Hamiltonian (5) maps onto itself under Fourier transformation, and all the eigenstates are non-degenerate, the eigenfunctions $\phi(x)$ must likewise map into itself under Fourier transformation (7),

$$\tilde{\phi}_n(x) = (-i)^n \phi_n(x). \tag{25}$$

This condition is directly fulfilled by certain functions, like the Gaussian eigenfunctions of the harmonic oscillator $H = \frac{1}{2}(k^2 + x^2)$,

$$\phi_n(x) = \left(x - \frac{\partial}{\partial x}\right)^n \exp\left(-\frac{x^2}{2}\right),$$

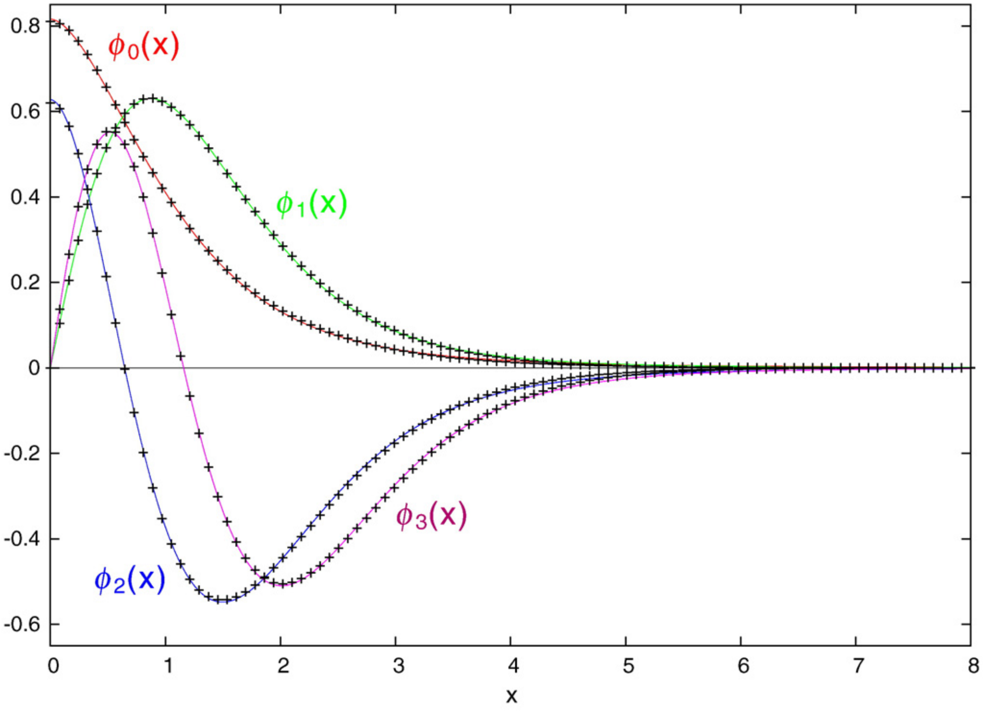

Fig. 3. Juxtapositions of the first four eigenfunctions $\phi_n(x)$ obtained numerically (lines) with the fits described in the text (black crosses).

or the function

$$\phi_0(x) = \frac{1}{\cosh}\left(\sqrt{\frac{\pi}{2}}\,x\right).$$

The eigenfunctions of Eq. (5), however, do not need to be of any such particular form. For example, the Ansatz

$$\phi_n(x) = i^n\,\tilde{\varphi}_n(x) + \varphi_n(x) \tag{26}$$

satisfies Eq. (25) in general, as Eq. (7) implies $\tilde{\tilde{\varphi}}_n(x) = \varphi_n(-x) = (-1)^n\varphi_n(x)$.

It is conceivable that the function $\varphi(x)$ displays the required asymptotic behavior mentioned above, while the Fourier transform $\tilde{\varphi}(x)$ falls off more rapidly. A first guess for the ground state along these lines might be

$$\varphi_0(x) = \frac{1}{(x^2 + a^2)^{3/2}}, \tag{27}$$

with its Fourier transform given by a modified Bessel function of the second kind,

$$\tilde{\varphi}_0(x) = \sqrt{\frac{2}{\pi}}\frac{|x|}{a}K_1(a|x|). \tag{28}$$

With $a \approx 1.172$, this provides a very reasonable approximation, but does not solve the problem exactly.

5.2. Asymptotic behavior

Even though we are unable to solve Eq. (11), we can use it to determine the asymptotic behavior of the solutions $\phi_n(x)$ as $x \to \infty$ accurately. Let us first consider even eigenfunctions $\phi_n(-x) = \phi_n(x)$. Then Eq. (11) becomes

$$\frac{1}{\pi}\frac{\partial}{\partial x}\mathcal{P}\int_0^\infty \frac{2x\phi_n(x')}{x^2 - x'^2}dx' + |x|\phi_n(x) = \lambda_n\phi_n(x), \tag{29}$$

For $x \to +\infty$, we obtain

$$-\frac{2}{\pi}\frac{1}{x^2}\int_0^\infty \phi_n(x')dx' + O\left(\frac{1}{x^4}\right) + (x - \lambda_n)\phi_n(x) = 0. \tag{30}$$

With Eqs. (7) and (25), however, we may write

$$\int_{-\infty}^{\infty} \phi_n(x)dx = \sqrt{2\pi}\tilde{\phi}_n(0) = (-i)^n\sqrt{2\pi}\phi_n(0), \tag{31}$$

and hence obtain for n even

$$\phi_n(x) = (-1)^{n/2}\sqrt{\frac{2}{\pi}}\phi_n(0)\left(\frac{1}{x^3} + \frac{\lambda_n}{x^4} + O\left(\frac{1}{x^5}\right)\right). \tag{32}$$

Similarly, we write Eq. (11) for the odd eigenfunctions $\phi_n(-x) = -\phi_n(x)$

$$\frac{1}{\pi}\frac{\partial}{\partial x}\mathcal{P}\int_0^\infty \frac{2x'\phi_n(x')}{x^2 - x'^2}dx' + |x|\phi_n(x) = \lambda_n\phi_n(x), \tag{33}$$

For $x \to +\infty$, we obtain

$$-\frac{4}{\pi}\frac{1}{x^3}\int_0^\infty x'\phi_n(x')dx' + O\left(\frac{1}{x^5}\right) + (x-\lambda_n)\phi_n(x) = 0 \tag{34}$$

With Eqs. (7) and (25), the integral becomes

$$\begin{aligned}\int_{-\infty}^{\infty} x\phi_n(x)dx &= \sqrt{2\pi}\cdot i\frac{\partial}{\partial k}\tilde{\phi}_n(k)\Big|_{k=0} \\ &= (-i)^{n-1}\sqrt{2\pi}\phi_n'(0).\end{aligned} \tag{35}$$

This yields for n odd

$$\phi_n(x) = (-1)^{\frac{(n-1)}{2}}2\sqrt{\frac{2}{\pi}}\phi_n'(0)\left(\frac{1}{x^4} + \frac{\lambda_n}{x^5} + O\left(\frac{1}{x^6}\right)\right). \tag{36}$$

The asymptotic behavior emphasizes how different the bi-linear oscillator (5) is from the well known harmonic oscillator.

5.3. Integral relations

We can apply some general properties of Hilbert transformations, defined as [8]

$$\mathcal{H}[f](x) \equiv \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{f(x')}{x-x'}dx', \tag{37}$$

where $\mathcal{P}$ denotes the principle part, to rewrite Eq. (11). With

$$\frac{\partial}{\partial x}\mathcal{H}[f](x) = \mathcal{H}\left[f'\right](x), \tag{38}$$

$$\mathcal{H}[\mathcal{H}[f]](x) = -f(x), \tag{39}$$

we obtain

$$\frac{\partial\phi_n(x)}{\partial x} + \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{(\lambda_n - |x'|)\phi_n(x')}{x-x'}dx' = 0. \tag{40}$$

Expanding the integral in the limit $x \to \infty$, we obtain for n even

$$\frac{\partial\phi_n(x)}{\partial x} = \frac{2}{\pi}\frac{1}{x}\int_0^\infty(\lambda_n - x)\phi_n(x)dx + O\left(\frac{1}{x^3}\right). \tag{41}$$

With Eq. (32), this implies

$$\int_0^\infty (x-\lambda_n)\phi_n(x)dx = 0, \tag{42}$$

and with Eq. (31)

$$\int_0^\infty x\phi_n(x)dx = (-1)^{n/2}\sqrt{\frac{\pi}{2}}\lambda_n\phi_n(0). \tag{43}$$

Similarly, we obtain in this limit for n odd

$$\frac{\partial\phi_n(x)}{\partial x} = \frac{2}{\pi}\frac{1}{x^2}\int_0^\infty x(\lambda_n - x)\phi_n(x)dx + O\left(\frac{1}{x^4}\right). \tag{44}$$

With Eq. (36), this implies

$$\int_0^\infty x(x-\lambda_n)\phi_n(x)dx = 0, \tag{45}$$

and with Eq. (35)

$$\int_0^\infty x^2\phi_n(x)dx = (-1)^{\frac{(n-1)}{2}}\sqrt{\frac{\pi}{2}}\lambda_n\phi_n(0). \tag{46}$$

6. Conclusion

We have succeeded in solving the bi-linear oscillator $H = v|p| + F|x|$ both quasi-classically and numerically. In an attempt to solve it analytically as well, we have derived a differential and integral equation, and obtained the asymptotic behavior for large x. We further formulated several conditions the solutions must satisfy. The problem of obtaining an analytical solution, however, is still open.

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