On the linear dispersion–linear potential quantum oscillator

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

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I. INTRODUCTION

With the quantum theory, as it was called at the time, nearing it first centennial anniversary, it is a rare opportunity to study an 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 a parameter, however, appears to provide an example.

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\(^2\). Spinons carry the spin of an electron but no charge. Since the antiparticle for a spinon is just another spinon with its spin reversed, the spectrum has only a positive energy branch. An one couples two chains antiferromagnetically\(^\perp\), the coupling \( J_4 \) will induce a linear confinement potential between pairs of spinons, as the rungs between two spinons become effectively decorrelated\(^3\). 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

\[
H = v|p| + F|x|, 
\]

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 \( \overset{\scriptscriptstyle{\dagger}}{H} \) are.

From dimensional considerations, it is immediately clear that they must scale like \( \sqrt{\hbar vF} \).

II. QUASICLASSICAL APPROACH

Even though the usual method of quantization can not be applied directly, the problem can still be approached quasi-classically. Applying the Bohr-Sommerfeld quantization condition\(^4\)

\[
\frac{1}{2\pi\hbar} \oint p dx = n + \frac{1}{2},
\]

where we are supposed to integrate over the entire classical orbit, results with \( p(x) = \frac{E_n - F|x|}{v} \) in

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

Carrying out the integration yields

\[
E_n = \sqrt{\pi \left( n + \frac{1}{2} \right) \cdot \sqrt{\hbar vF}}. 
\]

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.

III. 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

\[
H = |k| + |x|, 
\]

which is obtained from \( \overset{\scriptscriptstyle{\dagger}}{H} \) by rescaling

\[
\frac{H}{\sqrt{\hbar vF}} \to H, \quad \sqrt{\frac{\hbar vF}{F}} k \to k, \quad \text{and} \quad \sqrt{\frac{F}{\hbar v}} x \to x. 
\]

Let us denote the eigenvalues of \( \overset{\scriptscriptstyle{\dagger}}{H} \) by \( \lambda \) and the eigenfunctions by \( \phi(x) \). With

\[
\hat{\phi}(k) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(x) e^{-ikx} dx, 
\]

\[
\phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\phi}(k) e^{ikx} dk, 
\]

where \( k \) is the wave number.
we may write
\[ |k| \phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} k \text{sign}(k) e^{ikx} dk \]
\[ = -i \frac{\partial}{\partial x} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \text{sign}(k) e^{ikx} dk \]
\[ = -i \frac{\partial}{\partial x} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{s}(x - x') \phi(x') dx' \]
where
\[ \text{sign}(k) = \begin{cases} +1 & k \geq 0 \\ -1 & k < 0 \end{cases} \]
is the sign function and
\[ \tilde{s}(x) = \frac{1}{\sqrt{2\pi}} \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} \text{sign}(k) e^{-|k|} e^{ikx} dk \]
\[ = \frac{2i}{\sqrt{2\pi}} \lim_{\epsilon \to 0} \frac{x^2}{x^2 + \epsilon^2} \frac{2i}{\sqrt{2\pi}} \mathcal{P} \frac{1}{x} \]
where \( \mathcal{P} \) denotes the principal part, is the Fourier transform thereof. The eigenfunctions \( \phi(x) \) with eigenvalues \( \lambda \) are hence the solutions of
\[ \frac{1}{\pi} \frac{\partial}{\partial x} \mathcal{P} \int_{-\infty}^{\infty} \phi(x') dx' + |x| \phi(x) = \lambda \phi(x) \].

While \ref{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.

IV. NUMERICAL SOLUTION

To solve \ref{13} 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
\[ x_i = a \left( i - \frac{N + 1}{2} \right) \]
where \( i = 1, 2, \ldots, N \) and \( a \) is the lattice constant. The cutoff \( |x_c| = Na/2 \) in real space implies a cutoff
\[ \lambda_c = \frac{Na}{2} \]
for the potential energy in \ref{13}, which must be chosen significantly larger than the largest eigenvalue \( \lambda_n \) we wish to evaluate reliably. (From \ref{14}, we expect \( \lambda_n \) to be of order \( \sqrt{\pi (n + \frac{1}{2})} \).) On the other hand, the classically allowed part of the Hilbert space will contain only of the order of \( N/\lambda_c \) 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,
\[ |ak| = \frac{b_0}{2} + \sum_{m=1}^{\infty} b_m \cos(mak) \]
with
\[ b_m = \frac{1}{\pi} \int_{-\pi}^{\pi} dk |k| \cos(mk) = \begin{cases} \frac{\pi}{4} \frac{1}{m^2} & m = 0 \\ 0 & \text{otherwise,} \end{cases} \]
as one may easily verify through integration by parts. We proceed by writing \ref{14} in second quantized notation,
\[ H = \sum_k |k| c_k^\dagger c_k + \sum_i |x_i| c_i^\dagger c_i \]
\[ = \frac{1}{a} \sum_k |ak| c_k^\dagger c_k + a \sum_i \left| i - \frac{N + 1}{2} \right| c_i^\dagger c_i \]
where
\[ c_k^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{ikx_i} c_i^\dagger, \quad c_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-ikx_i} c_k. \]

Since
\[ \sum_k \cos(mak) c_k^\dagger c_k = \frac{1}{2} \sum_i (c_i^\dagger c_{i+m} + \text{h.c.}) \]
we obtain
\[ H = \sum_{i,j=1}^{N} c_i^\dagger h_{ij} c_j \]
with
\[ h_{ij} = \begin{cases} \frac{N}{2\lambda_c} \frac{\pi + 2\lambda_c}{2} |i - \frac{N + 1}{2}| & i = j \\ -\frac{N}{2\lambda_c} \frac{2}{(i-j)^2} & i - j \text{ odd} \\ 0 & \text{otherwise,} \end{cases} \]
where we have substituted \( \frac{2\lambda_c}{N} \) for \( a \).

Numerical diagonalization of \( h_{ij} \) yields the eigenvalues \( \lambda_n \) and eigenfunctions \( \psi_n(x_i) \) of \ref{13}, and hence the eigenvalues and eigenfunctions
\[ E_n = \lambda_n \sqrt{\hbar v F}, \quad \psi_n(x) = \phi_n \left( \sqrt{\frac{F}{\hbar v}} x \right) \]
of \ref{11}. The results for \( N = 20001, \lambda_c = 20 \) are listed in Table \ref{11} and Figures \ref{11} and \ref{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 \ref{11} we see that the quasi-classically obtained
The eigenvalues obtained numerically can be approximated by
\[ \phi_n(x) = x^n \exp\left(-a_n \sqrt{x^2 + b_n^2} + c_n\right) \] for \( n = 0, 1 \) and by
\[ \phi_n(x) = x^{n-2} \left(d_n^2 - x^2\right) \exp\left(-a_n \sqrt{x^2 + b_n^2} + c_n\right) \] for \( n = 2, 3 \), with parameters \( a_n, b_n, c_n, \) and \( d_n \) listed in Table I. Comparisons of these fits to the numerically obtained eigenfunctions are shown in Figure 3. The fits are not as good an approximation as Figure 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 \( x \to \infty \).

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 \( \lambda \)), 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 (20), this scattering is proportional to
\[ \int_{-\lambda - \lambda_t}^{\lambda + \lambda_t} \phi_n(x') \frac{dx'}{(x-x')^2} \propto \begin{cases} \frac{1}{x^2} & n \text{ even} \\ \frac{1}{x^3} & n \text{ odd} \end{cases} \] where \( \lambda_t \) is a cutoff to insure that we include the tail immediately surrounding the classically allowed region.

| \( n \) | \( \lambda_{2m} \) | \( \lambda_{2m+1} \) | \( \lambda_{3m} \) | \( \lambda_{3m+1} \) |
|------|----------------|----------------|----------------|----------------|
| 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         |

**FIG. 1:** (Color online) The first four symmetric eigenfunctions \( \phi_n(x) = \phi_n(x) \) for \( n \) even obtained numerically for \( N = 20001, \lambda_c = 20 \).

**TABLE I:** Eigenvalues \( \lambda_n \) for \( n = 0, \ldots, 19 \) obtained by exact diagonalization of (20) for \( N = 20001, \lambda_c = 20 \). From the scaling behavior with \( N \) and comparisons of different values for \( \lambda_n \), we estimate the error due to the finite size to be less than \( \pm 0.00002 \) for \( n \) even and \( \pm 0.00001 \) for \( n \) odd. For comparison, we also list the quasi-classical values (4).
TABLE II: Parameters obtained numerically from fitting (22) and (23) to the functions $\tilde{\phi}_n(x)$ obtained by exact diagonalization of (20) for $N = 20001$, $\lambda_e = 20$.

| $n$ | $a_n$ | $b_n$ | $c_n$ | $d_n$ |
|-----|-------|-------|-------|-------|
| 0   | 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 |

in the integral (from Figs. 11 and 24 we see that $\lambda_e = 3$ 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.

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.

V. FURTHER CONSIDERATIONS

It would be highly desirable to identify the exact eigenvalues and functions of (14). 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.

A. Fourier Symmetry

As the Hamiltonian (14) 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),

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

(25)

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

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

or the function

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

The eigenfunctions of (6), however, do not need to be of any such particular form. For example, the Ansatz

$$\phi_n(x) = i^n \tilde{\phi}_n(x) + \varphi_n(x)$$

(26)

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

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

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

(27)

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

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

(28)

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

B. Asymptotic Behavior

Even though we are unable to solve (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 (11) becomes

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

(29)

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

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

(30)

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

$$\int_0^\infty \phi_n(x) dx = \sqrt{2\pi} \tilde{\phi}_n(0) = (-i)^n \sqrt{2\pi} \phi_n(0),$$

(31)

and hence obtain for $n$ even

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

(32)

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

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

(33)

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

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

(34)

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

$$\int_{-\infty}^\infty x \phi_n(x) dx = \sqrt{2\pi} \cdot i \frac{\partial}{\partial k} \tilde{\phi}_n(k) \left|_{k=0}\right. = (-i)^{n-1} \sqrt{2\pi} \phi_n'(0).$$

(35)
This yields for $n$ odd
\[
\phi_n(x) = (-1)^{(n-1)/2} \sqrt{\frac{2}{\pi}} \phi_n(0) \left( \frac{1}{x^2} + \frac{\lambda_n}{x^4} + O\left(\frac{1}{x^6}\right) \right).
\] (36)

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

C. Integral relations

We can apply some general properties of Hilbert transformations, defined as
\[
\mathcal{H}[f](x) = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{f(x')}{x-x'} dx'.
\] (37)
where $\mathcal{P}$ denotes the principle part, to rewrite (11). With
\[
\frac{\partial}{\partial x} \mathcal{H}[f](x) = \mathcal{H}[f'](x),
\] (38)
\[
\mathcal{H}[\mathcal{H}[f]](x) = -f(x),
\] (39)
we obtain
\[
\frac{\partial \phi_n(x)}{\partial x} + \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{(\lambda_n - |x'|)\phi_n(x')}{x-x'} dx' = 0. \quad (40)
\]

Expanding the integral for the limit $x \to \infty$, we obtain for $n$ even
\[
\frac{\partial \phi_n(x)}{\partial x} = \frac{2}{\pi x} \int_0^{\infty} (\lambda_n - x')\phi_n(x') dx' + O\left(\frac{1}{x^6}\right). \quad (41)
\]

With (32), this implies
\[
\int_0^{\infty} (x - \lambda_n)\phi_n(x) dx = 0, \quad (42)
\]
and with (31)
\[
\int_0^{\infty} x\phi_n(x) dx = (-1)^{n/2} \sqrt{\frac{\pi}{2}} \lambda_n \phi_n(0). \quad (43)
\]

Similarly, we obtain in this limit for $n$ odd
\[
\frac{\partial \phi_n(x)}{\partial x} = \frac{2}{\pi x^2} \int_0^{\infty} x'(\lambda_n - x')\phi_n(x') dx' + O\left(\frac{1}{x^6}\right). \quad (44)
\]

With (36), this implies
\[
\int_0^{\infty} x(x - \lambda_n)\phi_n(x) dx = 0, \quad (45)
\]
and with (33)
\[
\int_0^{\infty} x^2\phi_n(x) dx = (-1)^{(n-1)/2} \sqrt{\frac{\pi}{2}} \lambda_n \phi_n(0). \quad (46)
\]

VI. 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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