A Ladder Operator Solution to the Particle in a Box Problem

Carl W. David Department of Chemistry University of Connecticut Storrs, Connecticut 06269-4060 (Dated: January 16, 2001)

A ladder operator solution to the particle in a box problem of elementary quantum mechanics is presented, although the pedagogical use of this method for this problem is questioned.

I. INTRODUCTION

Recent interest in ladder operators [1], and the curious omission from all current texts of the ladder operator solution to the particle in a box problem of elementary quantum mechanics makes one suspect that hidden in notes in various laboratories scattered all over the world are the details of why this particular approach, when applied to this particular problem, is not particularly pedagogically valid.

Were it otherwise, it would imply that no one has thought of applying this wonderful technique to what is the simplest of all quantum mechanical problems. Since it is inconceivable that persons teaching the ladder operator technique for harmonic oscillators [2], rigid rotors and angular momentum [3, 4], and the H-atom [5–7], etc., have not thought of this application, it must be that there is something curious about the problem that makes it of less than paramount interest.

For the precocious student, the one who asks radically different questions from the norm, the existence of a ladder operator in this particular problem should excite some interest. Here then is an approach to the ladder operator problem for the particle in a box in the domain $0 \le x \le L$ which possibly illustrates why the method has not gained universal acceptance for this problem. It appears to be related to that of Kais and Levine [8].

II. CONSTRUCTING THE LADDER OPERATOR

We start by remembering the trigonometric definition of the sine of the sum of two angles, i.e.,

$$\sin(\alpha + \beta) = \sin \alpha \cos \beta + \cos \alpha \sin \beta \tag{1}$$

We seek an operator, M^+ which takes a state $|n\rangle$ and ladders it up to the next state, i.e., $|n+1\rangle$. Since the particle in a box problem is already solved, i.e., we know that $|n\rangle$ is $\sin \frac{n\pi x}{L}$ we can employ this knowledge to construct our ladder operators. Symbolically, we define the up-ladder operator through the statement

$$M^+|n > \to |n+1 >$$

and we will require the inverse (the down-ladder operator), i.e.,

$$M^-|n > \rightarrow |n-1 >$$

where the down-ladder operator is lowering us from n to n-1 as usual.

One knows that there is a lower bound to the ladder, i.e., that one can not ladder down from the lowest state (n = 1), i.e.,

$$M^{-}|lowest >= 0$$

A. Form of the Up-Ladder and Down-Ladder Operators

What must the form of M^+ be, in order that it function properly? The up-ladder operator, M^+ , is defined according to

$$M^+\left(\sin\left(\frac{n\pi x}{L}\right)\right) \to \sin\left(\frac{(n+1)\pi x}{L}\right)$$
 (2)

which, using Equation 1 and $\alpha = \frac{n\pi x}{L}$ and $\beta = \frac{\pi x}{L}$ may be expressed as

$$M^{+} = \cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right) + \sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right)$$
(3)

i.e.,

$$M^{+}|n \rangle \rightarrow \cos\left(\frac{\pi x}{L}\right)|n \rangle + \left(\frac{L}{n\pi}\right)\sin\left(\frac{\pi x}{L}\right)\frac{\partial|n \rangle}{\partial x} = |n+1\rangle$$

The down operator is obtained in an analogous way,

$$\sin\left(\frac{(n-1)\pi x}{L}\right) = \cos\left(\frac{\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right) - \sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right)$$

making use of the even and odd properties of cosines and sines, respectively.

$$M^{-}|n\rangle \to \cos\left(\frac{\pi x}{L}\right)|n\rangle - \left(\frac{L}{n\pi}\right)\sin\left(\frac{\pi x}{L}\right)\frac{\partial|n\rangle}{\partial x} \to |n-1\rangle$$
$$M^{-} = \cos\left(\frac{\pi x}{L}\right) - \left(\frac{L}{n\pi}\right)\sin\left(\frac{\pi x}{L}\right)\frac{\partial}{\partial x}$$

The operators M^+ and M^- can be rewritten in coördinate-momentum language as

$$M^{+} = \cos\left(\frac{\pi x}{L}\right) - \left(\frac{L}{i\hbar n\pi}\right)\sin\left(\frac{\pi x}{L}\right)p_{x}$$
$$M^{-} = \cos\left(\frac{\pi x}{L}\right) + \left(\frac{L}{i\hbar n\pi}\right)\sin\left(\frac{\pi x}{L}\right)p_{x}$$
(4)

III. COMMUTATION OF LADDER OPERATORS WITH THE HAMILTONIAN

A. Elementary Commutators

We need $[p_x, \cos \frac{\pi x}{L}]$ and $[p_x, \sin \frac{\pi x}{L}]$:

$$[p_x, \cos\frac{\pi x}{L}] = \imath \hbar \frac{\pi}{L} \sin\left(\frac{\pi x}{L}\right) = p_x \cos\frac{\pi x}{L} - \cos\frac{\pi x}{L} p_x$$
$$[p_x, \sin\left(\frac{\pi x}{L}\right)] = -\imath \hbar \frac{\pi}{L} \cos\left(\frac{\pi x}{L}\right) = p_x \sin\left(\frac{\pi x}{L}\right) - \sin\left(\frac{\pi x}{L}\right) p_x$$

and $[p_x^2, \cos\left(\frac{\pi x}{L}\right)]$ (and its sine equivalent):

$$[p_x^2, \cos\left(\frac{\pi x}{L}\right)] = 2i\hbar \frac{\pi}{L} \sin\left(\frac{\pi x}{L}\right) p_x + \hbar^2 \left(\frac{\pi}{L}\right)^2 \cos\left(\frac{\pi x}{L}\right)$$
$$[p_x^2, \sin\left(\frac{\pi x}{L}\right)] = -2i\hbar \frac{\pi}{L} \cos\left(\frac{\pi x}{L}\right) p_x + \hbar^2 \left(\frac{\pi}{L}\right)^2 \sin\left(\frac{\pi x}{L}\right)$$

B. The Commutator of M^+ with H_{op}

Remembering that

$$H_{op} = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

after some effort, one has

$$[H, M^+] = -\frac{\hbar^2}{2m} \left(-\left(\frac{\pi}{L}\right)^2 (2n+1) M^+ + 2n\left(\frac{\pi}{L}\right)^2 \cos\left(\frac{\pi x}{L}\right) \right) - \frac{2}{n} \cos\left(\frac{\pi x}{L}\right) \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$
(5)

IV. LADDERING

Then, if

$$H|n\rangle = \epsilon_n|n\rangle$$

operating from the left with M^+ one has

$$M^+H|n\rangle = \epsilon_n M^+|n\rangle = \epsilon_n|n+1\rangle$$

and since $[H, M^+] = HM^+ - M^+H$, using Equation 5 one has

$$HM^+|n > -[H, M^+]|n > = \epsilon_n|n+1 >$$

$$H|n+1 > -[H, M^+]|n > = \epsilon_n|n+1 >$$

and then, after a tedious amount of algebra, one obtains

$$H|n+1> + \left[2n\left(\frac{\pi}{L}\right)^2 - \frac{4m}{n\hbar^2}\epsilon_n\right]\cos\left(\frac{\pi x}{L}\right)|n> = \epsilon_n|n+1> + \frac{\hbar^2}{2m}\left(\left(\frac{\pi}{L}\right)^2(2n+1)\right)|n+1>$$

From this we conclude that, if the elements in square brackets cancelled perfectly, $M^+|n+1 >$ would be an eigenfunction, i.e., if

$$\left[2n\left(\frac{\pi}{L}\right)^2 - \frac{4m}{n\hbar^2}\epsilon_n\right] = 0$$

i.e.,

$$\epsilon_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$

then

$$H|n+1\rangle = \left(\epsilon_n + \frac{\hbar^2}{2m}\left(\left(\frac{\pi}{L}\right)^2(2n+1)\right)\right)|n+1\rangle$$

$$=\frac{\hbar^2 \pi^2}{2mL^2} \left(n^2 + 2n + 1\right) |n+1\rangle = \frac{\hbar^2 \pi^2}{2mL^2} \left((n+1)^2\right) |n+1\rangle = \epsilon_{n+1} |n+1\rangle$$

This represents a deluge of results, since we have obtained the redundant result of the form of the eigenvalue and the form of the next (higher) eigenvalue. Generally, we have to work a bit harder in ladder operator solutions to quantum mechanical problems, than we have had to here.

V. DISCUSSION

Is it worthwhile to note the existence of this ladder operator approach? That curious students might worry about this obvious omission (or absence) prompts these remarks. But there is no question that the presentation implies a circularity of reasoning which, although it might exist in other problems, is never so self-evident. We are presupposing the existence and form of the eigenfunctions prior to attacking the problem. Had we started with the operators as postulated in Equation 2, the circularity of the argument would not have been so evident.

What is worth keeping here? It is clear that the current repertoire of exercises of evaluating commutators can be expanded to include examples other than x^n and p_x^m e.g., $[p_x, \sin x]$.

Also, what becomes clear in constructing the original ladder operator, is that the trigonometric formula for the sin of the sum of two angles makes the form possible. This implies that similar "addition" formulae lie at the fundament of the ladder operator approach in more common cases, which is, perhaps, enlightening.

In all, however, this ladder operator approach to the particle in a box problems probably deserves its own obscurity (or absence). No simplification occurs in carrying out this derivation which warrants expending the effort to lay the ground work for the derivation.

One concludes that the ladder operator exists, is interesting, but that its relevance to the teaching and learning processes lies somewhere in the venue of exercises.

It is a pleasure to acknowledge that the material presented here arose out of a discussion with Professor Jeffrey Bocarsly concerning Freshman Chemistry instruction. That no magic scheme for teaching this material to the mathematically unsophisticated absent traditional methods was found does not detract from the pleasure of having had the discussion.

- D. D. Fitts, J. Chem. Ed. **72**, 1066 (1995).
 L. U. R. Montemayor, Am. J. Phys. **51**, 641 (1983).
- [3] R. E. R. O. L. deLange, Am. J. Phys. 55, 913 (1987).
- [4] R. E. R. O. L. deLange, Am. J. Phys. 55, 950 (1987).
- [5] R. M. G. J. D. Newmarch, Am. J. Phys. 46, 658 (1978).
- [6] J. B. Boyling, Am. J. Phys. 56, 943 (1988).
- [7] C. W. David, Am. J. Phys. **34**, 984 (1966).
- [8] R. D. L. S. Kais, Phys. Rev. A 34, 4615 (1986).