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Why is it so difficult to generalize Heisenberg's matrix mechanics from the harmonic oscillator to other exactly solvable problems?

J. K. Freericks[a]

Department of Physics, Georgetown University, 37th and O Sts. NW, Washington 20057, DC, USA

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Abstract In 1925, Heisenberg, and later Born and Jordan, developed matrix mechanics as the first viable modern theory for quantum mechanics. While this approach worked beautifully for the simple harmonic oscillator and for angular momentum states, it was not able to solve other problems, which ultimately lost favor to the wavefunction approach of Schrödinger. In this article, I discuss why this was the case. In particular, I discuss how one can use similar techniques to what Heisenberg, Born and Jordan did to find the ground state and ground-state energy of all exactly solvable problems by properly factorizing the Hamiltonian into a positive semidefinite operator form. However, only by introducing an abstract vector space and abstract operators can one find all eigenvalues and eigenstates of these systems. I describe how one might have proceeded to do this using the matrix mechanics formalism. Along the way, I will describe, where the approach is limited and how one can advance past those limitations.

1 Introduction

Modern quantum mechanics was born in 1925 when Heisenberg discovered matrix mechanics [1]. In that work, Heisenberg showed how the properties of atomic spectra required one to work with matrices rather than functions, and soon thereafter, Born and Jordan showed how one can derive the canonical commutation relation in this matrix form [2]. The approach can be used to solve for the energy eigenvalues of the one-dimensional quantum harmonic oscillator. Heisenberg did this and corrected the Bohr–Sommerfeld quantization condition, which predicted an incorrect result for those energy levels.

However, matrix mechanics suffered in having difficulty solving other problems in quantum mechanics, especially finding the energy levels of hydrogen. While Pauli did solve this problem [3], his technique did not involve working directly with matrix elements but instead he discovered the SO(4) symmetry of hydrogen and used Lie algebraic methods to determine the spectrum.

Why was it so difficult to solve other problems with matrix mechanics? One can trace this to their need to find the momentum and position matrices and then using them to find the Hamiltonian in a diagonal form. Because these matrices are all infinite in size and because the equations are nonlinear matrix equations, this procedure is not easy to carry out (and we show precisely why below). Instead, what is possible is that one can factorize the Hamiltonian into a positive semi-definite form, which allows us to immediately find the ground-state energy. But then, one has to introduce the quantum states of the infinite-dimensional vector space to be able to ultimately solve these problems. However, this can be done using most of the matrix mechanics formalism. It is just a few technical issues that make some steps challenging to carry out in the matrix format (and requiring some *ad hoc* rules, as we will see below).

My approach to working through this material is not to follow a historical pathway. Instead, I employ the ideas of this approach, combined with more modern ideas, to see how far one can proceed. Along the way, I will describe why it is so difficult to generalize matrix mechanics, even when one uses more modern ideas.

[a] e-mail: james.freericks@georgetown.edu (corresponding author)

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2 Heisenberg's matrix mechanics

Atomic spectra satisfy the Rydberg–Ritz combination principle, which means the spectral line energies are given by the differences of energy levels of the atom. Heisenberg recognized that if he constructed matrices $\mathbf{M}_{mn}$ whose diagonal elements were time independent and whose off-diagonal elements depend on time via $\exp(i(E_m - E_n)t/\hbar)$, then it automatically allows for the inclusion of energy differences as the fundamental object of the theory. However, the real key came from examining the product of two matrices $\sum_l \mathbf{M}_{ml}\mathbf{N}_{ln} = (\mathbf{MN})_{mn}$ and noticing that the product satisfies the same dependence on energies due to the fact that $E_m - E_l + E_l - E_n = E_m - E_n$. This means all objects constructed from these matrices, including functions of the matrices, will have the same time dependence on the energies for the off-diagonal matrix elements.

If we proceed in a modern perspective [4], we next require these matrices to satisfy the Hamilton equations of motion in order for them to be able to reduce to the classical results in some fashion. This requirement is the equivalent of Ehrenfest's theorem, but taken here as a postulate. We work with time-independent Hamiltonians only, and we make the assumption (correct for one-dimensional problems on the full domain) that the energy eigenvalues are nondegenerate). The formalism starts from the Hamiltonian, which takes the form (as an infinite-dimensional matrix) given by

$$\mathbf{H}_{mn} = \left(\frac{1}{2M}\mathbf{P}^2 + V(\mathbf{Q})\right)_{mn}, \tag{1}$$

where $\mathbf{P}$ is the momentum matrix and $\mathbf{Q}$ is the position matrix. $V(\mathbf{Q})$ is a matrix-valued function that represents the potential energy. The mass is M. Note that the relationship between the $\mathbf{P}$ and $\mathbf{Q}$ matrices and the Hamiltonian is a nonlinear relation.

In the Heisenberg approach, the Hamiltonian must be a diagonal matrix, because it is time independent (from a modern perspective, it is the Hamiltonian matrix expressed in its time-dependent energy eigenstate basis, which is obviously diagonal and time-independent). Hence, it is a diagonal matrix $\mathbf{H}_{mn} = E_n\delta_{mn}$; we usually order the basis, so that $E_0 < E_1 < \cdots$ and the ground state is the 0 index. A general matrix $\mathbf{M}$ has a matrix element given by $\mathbf{M}_{mn} = C_{mn}\exp(\frac{i}{\hbar}(E_m - E_n)t)$, with C_{mn} a number, so one can immediately derive the Heisenberg equation of motion, because

$$\dot{\mathbf{M}}_{mn} = \frac{i}{\hbar}(E_m - E_n)\mathbf{M}_{mn} = \tfrac{i}{\hbar}[\mathbf{H}, \mathbf{M}]_{mn}, \tag{2}$$

where the square brackets denote the commutator, which satisfies $[\mathbf{M}, \mathbf{N}] = \mathbf{MN} - \mathbf{NM}$. Heisenberg recognized that the commutator of position with momentum was an important object to consider in the theory. He also recognized that matrices of position, momentum and the potential are Hermitian.

I next show that the commutator is independent of time using the Hamilton equations of motion ($\dot{\mathbf{Q}} = \mathbf{P}/M$ and $\dot{\mathbf{P}} = -V'(\mathbf{Q})$) as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathbf{Q}, \mathbf{P}] = [\dot{\mathbf{Q}}, \mathbf{P}] + [\mathbf{Q}, \dot{\mathbf{P}}] = \frac{1}{M}[\mathbf{P}, \mathbf{P}] - [\mathbf{Q}, V'(\mathbf{Q})] = 0, \tag{3}$$

because $\mathbf{P}$ commutes with itself, and $\mathbf{Q}$ must commute with any function of $\mathbf{Q}$ (this can easily be established by expanding the potential in a power series in $\mathbf{Q}$). Therefore, because the canonical commutation relation is time-independent, it must be diagonal, or $[\mathbf{Q}, \mathbf{P}]_{mn} = \mathbf{C}_m\delta_{mn}$.

To determine the precise value for the canonical commutation relation, I proceed as follows:

$$\mathbf{P} = M\dot{\mathbf{Q}} = \frac{iM}{\hbar}[\mathbf{H}, \mathbf{Q}] = -\frac{i}{2\hbar}(\mathbf{P}[\mathbf{Q}, \mathbf{P}] + [\mathbf{Q}, \mathbf{P}]\mathbf{P}), \tag{4}$$

where I used the Leibniz product rule for the commutator and the fact that the commutator is odd upon interchanging its elements. Taking the matrix elements of the final result in Eq. (4), one finds that $i\hbar\mathbf{P}_{mn} = \frac{1}{2}(\mathbf{C}_m + \mathbf{C}_n)\mathbf{P}_{mn}$. This tells us that the average of any two matrix elements of the canonical commutation relation is equal to $i\hbar$ for any two indices, where $\mathbf{P}_{mn} \neq 0$. To find the specific value, we need to note two more facts. First, we require the canonical commutation relation to be independent of the Hamiltonian and second, the diagonal basis for one Hamiltonian is a different diagonal basis for another Hamiltonian. These two facts require the diagonal matrix of the canonical commutation relation to be unchanged when an arbitrary change of basis is applied to it. The only matrix that does this is the identity matrix, so we find that $[\mathbf{Q}, \mathbf{P}] = i\hbar\mathbf{I}$. Note how the canonical commutation relation is derived simply from the fact that the atomic spectra is given by energy differences and the correspondence principle is given by the Ehrenfest theorem.

Next, I show how the solution for the harmonic oscillator works. The Hamiltonian is

$$\mathbf{H} = \frac{1}{2M}\mathbf{P}^2 + \frac{1}{2}M\omega^2\mathbf{Q}^2 \tag{5}$$

and then the equations of motion give

$$\ddot{\mathbf{Q}} = \frac{\mathrm{d}}{\mathrm{d}t}\dot{\mathbf{Q}} = \frac{1}{M}\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{P} = \frac{1}{M}\frac{i}{\hbar}[\mathbf{H}, \mathbf{P}] = \frac{1}{2}\frac{i}{\hbar}\omega^2[\mathbf{Q}^2, \mathbf{P}] = -\omega^2\mathbf{Q}. \tag{6}$$

However, the second derivative of the $\mathbf{Q}_{mn}$ matrix element is also given by $-\omega_{mn}^2\mathbf{Q}_{mn}$, with $\omega_{mn} = (E_m - E_n)/\hbar$. Hence, we have

$$(\omega^2 - \omega_{mn})\mathbf{Q}_{mn} = (\omega - \omega_{mn})(\omega + \omega_{mn})\mathbf{Q}_{mn} = 0. \tag{7}$$

This implies that $\mathbf{Q}_{mn} = 0$ except when $E_m = E_n \pm \hbar\omega$. Because of the nondegenerate nature of the spectrum, this also implies the position matrix has at most two nonzero matrix elements in each column or row.

However, the lowest energy level, the ground state, cannot have any energy lower than it, so there is only one nonzero element in the zeroth row (and similarly for the zeroth column). This allows us to directly compute the ground-state energy. We examine the diagonal element of the canonical commutation relation, given by

$$\sum_n(\mathbf{Q}_{mn}\mathbf{P}_{nm} - \mathbf{P}_{mn}\mathbf{Q}_{nm}) = 2Mi\sum_n \omega_{nm}|\mathbf{Q}_{mn}|^2 = i\hbar, \tag{8}$$

after writing $\mathbf{P} = M\dot{\mathbf{Q}}$ and computing the time derivative from the explicit time dependence of the matrix. This also uses the fact that the position matrix is Hermitian. Choosing $m = 0$ has just one nonzero element in the summation, so I find that

$$|\mathbf{Q}_{01}|^2 = \frac{\hbar}{2M\omega} \quad \text{and similarly that} \quad |\mathbf{P}_{01}|^2 = \frac{\hbar M\omega}{2}. \tag{9}$$

Then, I can compute

$$\mathbf{H}_{00} = \frac{1}{2M}|\mathbf{P}_{01}|^2 + \frac{1}{2}M\omega^2|\mathbf{Q}_{01}|^2 = \frac{\hbar\omega}{2}, \tag{10}$$

which is the ground-state energy. Finally, because $E_m = E_n \pm \hbar\omega$, we discover that the nth energy level is $\hbar\omega(n + \frac{1}{2})$. One can also compute the full position and momentum matrices from this, but I do not go through those details here, because they are not needed.

3 Ladder operator formalism and factorization

The previous derivation looks nothing like the common approach given in textbooks, where ladder operators are used. The idea for the ladder operator came from Jordan and Pauli [5] and was incorporated in Born and Jordan's textbook [6] well before Dirac included it in his textbook [7]. The easiest way to work with this is to think of it as a method to factorize the Hamiltonian, which is a concept that was developed by Schrödinger in the 1940s [8].

The general strategy is to write

$$\mathbf{A} = \frac{1}{\sqrt{2M}}(\mathbf{P} - iW(\mathbf{Q})) \quad \text{and} \quad \mathbf{A}^\dagger = \frac{1}{\sqrt{2M}}(\mathbf{P} + iW(\mathbf{Q})), \tag{11}$$

with W a real-valued function, often called the superpotential. Here, † is the symbol for the Hermitian conjugate of the matrix, found by taking the transpose and complex conjugate of the original matrix. The fact that the superpotential is real is required for the two matrices to be Hermitian conjugates of each other. Then, when I compute $\mathbf{A}^\dagger\mathbf{A}$, I find

$$\mathbf{A}^\dagger\mathbf{A} = \frac{1}{2M}\mathbf{P}^2 + \frac{1}{2M}W^2(\mathbf{Q}) - \frac{i}{2M}[\mathbf{P}, W(\mathbf{Q})]. \tag{12}$$

For the harmonic oscillator, I choose $W(\mathbf{Q}) = M\omega\mathbf{Q}$, and find that

$$\mathbf{A}^\dagger\mathbf{A} = \frac{1}{2M}\mathbf{P}^2 + \frac{1}{2}M\omega^2\mathbf{Q}^2 - \frac{1}{2}\hbar\omega \quad \text{or} \quad \mathbf{H} = \mathbf{A}^\dagger\mathbf{A} + \frac{1}{2}\hbar\omega, \tag{13}$$

which is the standard result when expressed in terms of operators—here, of course the objects are infinite-dimensional matrices. Note that the ladder operators used here are just rescaled from the conventional definition. Working out the explicit relation is left to the reader.

The matrix $\mathbf{A}^\dagger\mathbf{A}$ is a positive semi-definite matrix, so its eigenvalues are all larger than or equal to 0. Hence, the minimal eigenvalue of the Hamiltonian is given by the constant, or $\frac{1}{2}\hbar\omega$, which is indeed the ground-state energy. Even when Jordan and Pauli found this factorization, they did not recognize the positive semidefinite nature of the matrix and so they did not work with it in this way.

Indeed, one cannot complete the derivation to find other energy eigenvalues at this stage, because there are no states to work with. Instead, we need to continue to use methods such as those described in the previous section to find the higher energy eigenvalues. I will describe how to introduce states and make a more modern argument in the next section.

What about other systems? There are two ways to proceed. First, one can pick any appropriate superpotential W and use a similar calculation as above to determine the potential and the ground state energy. Second, one can start from the potential and try to find a superpotential that can be used to factorize the problem. While the first approach seems to be very attractive, it turns out that there are requirements on the function W, such as it should not diverge anywhere inside the domain and it needs to be positive as its argument approaches positive infinity and negative as it approaches negative infinity if we want to use it to determine all of the energy eigenvalues using a procedure described in the next section. There does not seem to be any way to justify those conditions at the matrix-mechanics level, which is a drawback of this approach, because it requires working with wavefunctions to fully justify them (the conditions are related to normalizability of the quantum state and to the node theorem for the wavefunction). For example, you can see that if we chose the superpotential with the opposite sign than the one we used for the harmonic oscillator, then we would have found the ground state energy of the oscillator is $-\hbar\omega/2$, which is clearly incorrect, as no energy can be smaller than the minimum of the potential, or zero in this case. Of course this is not inconsistent with what a positive semidefinite matrix is, it just shows that in that case, the lowest energy eigenvalue is not a physical one. What it does do is point to the fact that if you wanted to use factorization to find the ground-state energy, then you need to know the rules for the superpotential to do it correctly. This is a point often ignored in conventional instruction. When he introduced factorization, Schrödinger did introduce an *ad hoc* rule that if there was any ambiguity in the procedure always pick the choice that gives the highest energy. While such a rule would resolve the harmonic oscillator issue, Schrödinger never gave a reason for the rule, and I cannot find one to justify it, even though both Green [9] and Ohanian [10] have used that rule in developing the factorization method in their texts.

There are many known potentials that can be factorized in this way. All so-called shape-invariant potentials will work, but other choices can also work, even superpotentials that violate the above rule, such as $\alpha\mathbf{Q}^2$, if all one wants is to find one of the energy levels (which will be the ground state if the superpotential is nonsingular). Therefore, it seems like this approach lacks the needed guidance to produce correct results. Nevertheless, these points were missed by the pioneers, even though they knew how to factorize the harmonic oscillator as early as 1928. It is not clear why they did not proceed further with such an approach.

The way that Heisenberg, Born, and Jordan tried to solve their problems instead was to find other potentials, where they could determine $\mathbf{Q}$ and then $V(\mathbf{Q})$ and $\mathbf{P}$ to ultimately show how $\mathbf{H}$ is diagonal. This ends up being exceedingly difficult, because other problems do not have as simple an equation of motion as in Eq. (7) for the simple harmonic oscillator. Instead, one finds an equation of motion of the form $-\omega_{mn}^2\mathbf{Q}_{mn} = -\frac{1}{M}V'(\mathbf{Q})_{mn}$, which does not seem to have any clear way to simplify it, allowing either $\mathbf{Q}$ or $V(\mathbf{Q})$ matrices to be found. In fact, it is a nonlinear equation in infinite-dimensional matrices—clearly a challenge to figure out how to solve it.

Factorization does still work, if we pick the correct superpotential. Let us examine one example, the Morse potential is given by

$$V_{\text{Morse}}(\mathbf{Q}) = D_e\Big(e^{-2a(\mathbf{Q}-q_e)} - 2e^{-a(\mathbf{Q}-q_e)}\Big), \tag{14}$$

and is solved with a superpotential given by

$$W(\mathbf{Q}) = \sqrt{2MD_e}\left(1 - \frac{\hbar a}{2\sqrt{2MD_e}} - e^{-a(\mathbf{Q}-q_e)}\right), \tag{15}$$

which is positive for the argument going to $+\infty$, and negative for the argument going to $-\infty$, so it satisfies the superpotential rules. Then, we have

$$\mathbf{H} = \mathbf{A}^\dagger \mathbf{A} - D_e + \hbar a \sqrt{\frac{D_e}{2M}} - \frac{\hbar^2 a^2}{8M}. \tag{16}$$

Because of the positive definite nature of the matrices, one can read off the ground state energy as

$$E_{\text{gs}} = -D_e + \hbar a \sqrt{\frac{D_e}{2M}} - \frac{\hbar^2 a^2}{8M}. \tag{17}$$

Indeed, this is the correct ground state energy of the Morse potential.

Another example is the trigonometric Pöschl–Teller potential, of the form

$$V_{\text{PT}}(\mathbf{Q}) = \frac{\hbar^2 k(k+\frac{\pi}{L})}{2M} \sec^2\left(\frac{\pi \mathbf{Q}}{L}\right), \tag{18}$$

with $k > 0$ a real wavenumber and which has a domain that ranges from $-\frac{L}{2}$ to $\frac{L}{2}$. The correct superpotential is $W(\mathbf{Q}) = \hbar\big(k+\frac{\pi}{L}\big)\tan\Big(\frac{\pi \mathbf{Q}}{L}\Big)$, which diverges at the boundary of the domain, and from which one can directly compute that $\mathbf{H} = \mathbf{A}^\dagger \mathbf{A} + \hbar^2\big(k+\frac{\pi}{L}\big)^2/2M$, yielding the ground-state energy from the constant term. The divergence of superpotential at the edges of the domain is what is needed for the boundary condition to be consistent with the potential being $+\infty$ outside the domain, although it is not clear why this is so from the matrix-based approach. While I did not mention it, the other sign of the superpotential could have been used (with $k \to k - \frac{\pi}{L}$) to produce the same potential, but it has a lower energy, and Schrödinger's rule tells us to pick the one picked, which is the correct choice, as we will learn below.

Therefore, there are challenges with using this approach, and one can use Schrödinger's criterion, to maximize the ground-state energy, as a rule to do it properly (but there is no clear justification for this rule, except that it works *a posteriori*).

4 Introducing quantum states to complete the solution

Of course, we are interested in getting all of the energies not just the ground state, so we have to go outside of traditional matrix mechanics to proceed further. This is done using abstraction and linear algebra.

We have to recognize that these matrices are the representations of abstract operators in an infinite-dimensional vector space, and the basis Heisenberg chose is that of the time-evolving energy eigenbasis for the Hamiltonian. We can still work with the matrices and concrete vectors, instead of the abstract operators and abstract state vectors if we want, but the key insight is that we need to think in terms of state vectors as being an important object in addition to just the matrices themselves. This is a significant leap from the original discovery, but it becomes somewhat obvious, once Schrödinger showed the relationship between wave mechanics and matrix mechanics in 1926 [11].

In keeping with the spirit of matrix mechanics, I will continue to work in the time-dependent energy eigenbasis of the original Hamiltonian. It makes the analysis a bit more cumbersome, but I will show how it works below.

The key to this is defining auxiliary Hamiltonians from the factorized form of the original Hamiltonian and using what is called the intertwining relation. Being able to carry out this approach algebraically (via a matrix-mechanics approach), requires us to work with exactly solvable problems only, implying we must use so-called shape-invariant potentials. The only thing we need to know about these potentials is that the superpotential for the whole family always has the same functional form—just the numbers used in that functional form vary for subsequent factorizations. This will all become clear shortly.

The idea for proceeding in this fashion comes from Schrödinger in 1940 when he developed the factorization method [8]. The strategy is to create a factorization chain, and from this chain, one can read off the energy eigenvalues and energy eigenstate vectors.

I start from the factorized form of the original Hamiltonian, which is written as

$$\mathbf{H}_0 = \mathbf{A}_0^\dagger \mathbf{A}_0 + E_0 = \frac{\mathbf{P}^2}{2M} + V_0(\mathbf{Q}), \tag{19}$$

where I use the zero index for the first Hamiltonian in the chain. Then, I define the first auxiliary Hamiltonian with reversed ladder operators to be

$$\mathbf{H}_1 = \mathbf{A}_0\mathbf{A}_0^\dagger + E_0 = \frac{\mathbf{P}^2}{2M} + V_1(\mathbf{Q}), \tag{20}$$

with $V_1(\mathbf{Q}) = V_0(\mathbf{Q}) + [\mathbf{A}_0, \mathbf{A}_0^\dagger]$, which is typically a new potential, given by $V_0(\mathbf{Q}) + \frac{i}{M}[\mathbf{P}, W(\mathbf{Q})]$. To determine the next raising and lowering operator in the factorization chain, one must factorize the first auxiliary Hamiltonian via

$$\mathbf{H}_1 = \mathbf{A}_1^\dagger\mathbf{A}_1 + E_1 = \frac{\mathbf{P}^2}{2M} + V_1(\mathbf{Q}), \tag{21}$$

which can be a challenging task to complete. As mentioned above, for exactly solvable Hamiltonians, the new ladder operators have the same form as the old ones, with constants changed in them. This will become clear, as we proceed. Note, for physical solutions, we always find $E_1 > E_0$.

We simply continue the process by defining

$$\mathbf{H}_{i+1} = \mathbf{A}_i\mathbf{A}_i^\dagger + E_i = \frac{\mathbf{P}^2}{2M} + V_i(\mathbf{Q}), \tag{22}$$

which is then refactorized as

$$\mathbf{H}_{i+1} = \mathbf{A}_{i+1}^\dagger\mathbf{A}_{i+1} + E_{i+1} = \frac{\mathbf{P}^2}{2M} + V_{i+1}(\mathbf{Q}) \tag{23}$$

and again $E_{i+1} > E_i$. This creates what is called the factorization chain of Hamiltonians and energies.

We will need to find the ground states of each auxiliary Hamiltonian. These are vectors $\phi^{(i)}$ that satisfy $\sum_n (\mathbf{A}_i)_{mn}\phi_n^{(i)} = 0$, that is, we need to find a concrete vector $\phi^{(i)}$ that is in the null space of the matrix $\mathbf{A}_i$. There is only one physical null vector for each of our Hamiltonians. What is surprising, is that to obtain the spectra, we do not need to find the concrete expression for these vectors, we need only know that they exist. This is again a weak point of the matrix mechanics approach, because I cannot easily prove that they do exist, whereas using wave mechanics, the existence is part of the so-called node theorem [12]. These auxiliary ground-state vectors are required to be normalized to equal 1, so that $\sum_m |\phi_m^{(i)}|^2 = 1$

Next, we see that these two definitions for the auxiliary Hamiltonians allow us to derive the so-called intertwining relation given by

$$\mathbf{H}_i\mathbf{A}_i^\dagger = \Big(\mathbf{A}_i^\dagger\mathbf{A}_i + E_i\Big)\mathbf{A}_i^\dagger = \mathbf{A}_i^\dagger\Big(\mathbf{A}_i\mathbf{A}_i^\dagger + E_i\Big) = \mathbf{A}_i^\dagger\mathbf{H}_{i+1}. \tag{24}$$

Hence, I can move $\mathbf{A}_i^\dagger$ past $\mathbf{H}_i$ from right to left, and have the index of the Hamiltonian increase by 1.

This then allows us to construct the ith excited state of our original Hamiltonian (unnormalized) as follows:

$$\psi_m^{(i)} = \sum_n \Big(\mathbf{A}_0^\dagger\mathbf{A}_1^\dagger\cdots\mathbf{A}_{i-1}^\dagger\Big)_{mn}\phi_n^{(i)}, \tag{25}$$

where I denote the eigenstates of the original Hamiltonian via ψ. The proof of this uses the intertwining relation. I multiply the energy eigenstate from the left by $\mathbf{H}_0$, to find

$$\begin{aligned}
\Big(\mathbf{H}_0\psi^{(i)}\Big)_m &= \sum_n \Big(\mathbf{H}_0\mathbf{A}_0^\dagger\mathbf{A}_1^\dagger\cdots\mathbf{A}_{i-1}^\dagger\Big)_{mn}\phi_n^{(i)} = \sum_n \Big(\mathbf{A}_0^\dagger\mathbf{H}_1\mathbf{A}_1^\dagger\cdots\mathbf{A}_{i-1}^\dagger\Big)_{mn}\phi_n^{(i)} \\
&\vdots \\
&= \sum_n \Big(\mathbf{A}_0^\dagger\mathbf{A}_1^\dagger\cdots\mathbf{A}_{i-1}^\dagger\mathbf{H}_i\Big)_{mn}\phi_n^{(i)} = \sum_n \Big(\mathbf{A}_0^\dagger\mathbf{A}_1^\dagger\cdots\mathbf{A}_{i-1}^\dagger E_i\Big)_{mn}\phi_n^{(i)} \\
&= E_i\sum_n \Big(\mathbf{A}_0^\dagger\mathbf{A}_1^\dagger\cdots\mathbf{A}_{i-1}^\dagger\Big)_{mn}\phi_n^{(i)} = E_i\psi_m^{(i)}.
\end{aligned} \tag{26}$$

In this derivation, the intertwining relation is employed to move the Hamiltonian from left to right, one-by-one, ending with $\mathbf{H}_i$, for which $\phi^{(i)}$ is the ground-state eigenvector. Hence, I have shown that the state I created is indeed an excited energy eigenstate of the original Hamiltonian. This further implies that each energy found in the factorization chain (after E_0) is an excited energy level of the original Hamiltonian. Being able to show this is why we defined the auxiliary Hamiltonians as we did.

One can use intertwining to find the normalized energy eigenstate. This is done by first forming

$$\sum_m |\psi_m^{(i)}|^2 = \sum_{mn} \phi_m^{(i)*} \Big(\mathbf{A}_{i-1} \cdots \mathbf{A}_1 \mathbf{A}_0 \mathbf{A}_0^\dagger \mathbf{A}_1^\dagger \cdots \mathbf{A}_{i-1}^\dagger \Big)_{mn} \phi_n^{(i)}. \tag{27}$$

Next, I note that the innermost product of ladder operators is of the form $\mathbf{A}_0 \mathbf{A}_0^\dagger = \mathbf{H}_1 - E_0 \mathbf{I}$. I then use intertwining to move this Hamiltonian matrix minus a constant times the identity all the way to the right, where it becomes $\mathbf{H}_i - E_0 \mathbf{I}$. Then, I act the Hamiltonian against its eigenstate, where it is replaced by E_i. This can then be factored out of the expression and I have

$$\sum_m |\psi_m^{(i)}|^2 = (E_i - E_0) \sum_{mn} \phi_m^{(i)*} \Big(\mathbf{A}_{i-1} \cdots \mathbf{A}_1 \mathbf{A}_1^\dagger \cdots \mathbf{A}_{i-1}^\dagger \Big)_{mn} \phi_n^{(i)}, \tag{28}$$

which removed two matrices from the center and replaced them by the difference of two energy eigenvalues. I then repeat the process. The next term has $\mathbf{A}_1 \mathbf{A}_1^\dagger = \mathbf{H}_2 - E_1 \mathbf{I}$, and I proceed as before obtaining the numerical factor $E_i - E_1$. I then repeat until all raising and lowering matrices are removed and I have

$$\sum_m |\psi_m^{(i)}|^2 = (E_i - E_0)(E_i - E_1) \cdots (E_i - E_{i-1}) \sum_m |\phi^{(i)}|_m^2, \tag{29}$$

so, we find that the normalized ith excited state of $\mathbf{H}_0$ is

$$\psi_m^{(i)} = \sum_n \frac{\Big(\mathbf{A}_0^\dagger \mathbf{A}_1^\dagger \cdots \mathbf{A}_{i-1}^\dagger \Big)_{mn} \phi_n^{(i)}}{\sqrt{(E_i - E_0)(E_i - E_1) \cdots (E_i - E_{i-1})}}, \tag{30}$$

because the $\phi^{(i)}$ vector is normalized.

I want to reiterate that the factorizations themselves allow us to find the eigenvalues without the eigenstates, just as what was done in the original matrix-mechanics solution for the harmonic oscillator. Indeed, each of the energies found in the factorization chain is an energy eigenvalue of the original Hamiltonian matrix and those energies are all of the bound-state energies. However, if we use the ladder operators and the auxiliary Hamiltonian ground state properties, we can also calculate a number of different types of expectation values as well, without ever needing to explicitly determine any of the ground-state vectors or wavefunctions. An example of this is the Kramers–Pasternak relations which create and solve recurrence relations for the expectation values of powers of the radial matrix in energy eigenstates [13–15]. It is precisely, because all we need to know is the existence of these auxiliary ground state vectors and that they are annihilated by the corresponding lowering operator, which allows calculations of the spectrum to be done in the same fashion as the original matrix mechanics calculations and expectation values.

I now show how to construct the factorization chain for the two examples I gave before. We start with the Morse potential. Because it is a shape-invariant potential, I have

$$\mathbf{A}_j = \tfrac{1}{\sqrt{2M}} \Big(\mathbf{P} - i\sqrt{2MD_e} \Big(1 + \alpha_j - e^{-a(\mathbf{Q} - q_e)} \Big) \Big), \tag{31}$$

with α_j a number, yet to be determined. I can compute directly that

$$\begin{aligned} \mathbf{A}_j^\dagger \mathbf{A}_j = {} & \frac{\mathbf{P}^2}{2M} + D_e e^{-2a(\mathbf{Q}-q)} - D_e \Big(2(1-\alpha_j) + \frac{\hbar a}{\sqrt{2MD_e}} \Big) e^{-a(\mathbf{Q}-q)} \\ & + D_e (1-\alpha_j)^2, \end{aligned} \tag{32}$$

and

$$\mathbf{A}_j \mathbf{A}_j^\dagger = \frac{\mathbf{P}^2}{2M} + D_e e^{-2a(\mathbf{Q}-q)} - D_e \Big(2(1-\alpha_j) - \frac{\hbar a}{\sqrt{2MD_e}} \Big) e^{-a(\mathbf{Q}-q)}$$

$$+ D_e(1-\alpha_j)^2. \tag{33}$$

I use both of these results to now find the specific ladder operators and energies for the factorization chain.

Starting with the first factorization, where we already showed that $\alpha_0 = \hbar a/\sqrt{8MD_e}$ and $E_0 = -D_e + \hbar a\sqrt{D_e}/\sqrt{2M} - \hbar^2 a^2/8M$, we now compute V_1 to be

$$V_1(\mathbf{Q}) = D_e e^{-2a(\mathbf{Q}-q)} - 2\left(1 - \frac{\hbar a}{\sqrt{2MD_e}}\right)e^{-a(\mathbf{Q}-q)} \tag{34}$$

and find that

$$\alpha_1 = \frac{3\hbar a}{\sqrt{8MD_e}} \quad \text{and} \quad E_1 = -D_e + 3\hbar a\sqrt{\frac{D_e}{2M}} - \frac{9\hbar^2 a^2}{8M}. \tag{35}$$

Continuing in this fashion, we find that

$$\alpha_n = \frac{(2n+1)\hbar a}{\sqrt{8MD_e}} \quad \text{and} \quad E_n = -D_e + (2n+1)\hbar a\sqrt{\frac{D_e}{8MD_e}} - \frac{(2n+1)^2\hbar^2 a^2}{8M}. \tag{36}$$

By looking at the potential, we see that if $n > \sqrt{2MD_e}/\hbar a$, then the auxiliary potential at the nth step of the factorization chain has no minimum, so it cannot have a bound state anymore. Indeed, when n first satisfies the inequality above, the factorization chain must terminate, and there are no more bound states. The condition is somewhat more stringent than does the potential have a minimum and it is actually given by $n > \sqrt{2MD_e}/\hbar a - \frac{1}{2}$. Above the bound states, we have the continuum for $E > 0$. There is no clear way to determine the continuum states via factorization in a matrix mechanics form, because it requires the proper application of boundary conditions to solve the problem.

The second example will be the trigonometric Pöschl–Teller potential. Using the general form of the superpotential, given by $W_j(\mathbf{Q}) = \hbar\left(k_j + \frac{\pi}{L}\right)\tan\left(\frac{\pi\mathbf{Q}}{L}\right)$, I then have

$$\mathbf{A}_j^\dagger \mathbf{A}_j = \frac{\mathbf{P}^2}{2M} + \frac{\hbar^2 k_j\left(k_j + \frac{\pi}{L}\right)}{2M}\sec^2\left(\frac{\pi\mathbf{Q}}{L}\right) - \frac{\hbar^2\left(k_j + \frac{\pi}{L}\right)^2}{2M}, \tag{37}$$

and

$$\mathbf{A}_j \mathbf{A}_j^\dagger = \frac{\mathbf{P}^2}{2M} + \frac{\hbar^2\left(k_j + \frac{\pi}{L}\right)\left(k_j + \frac{2\pi}{L}\right)}{2M}\sec^2\left(\frac{\pi\mathbf{Q}}{L}\right) - \frac{\hbar^2\left(k_j + \frac{\pi}{L}\right)^2}{2M}. \tag{38}$$

Now, starting with the potential in Eq. (18), I have $k_0 = k$ and $E_0 = \hbar^2\left(k + \frac{\pi}{L}\right)^2/2M$. I then find that

$$V_1(\mathbf{Q}) = \frac{\hbar^2\left(k + \frac{\pi}{L}\right)\left(k + \frac{2\pi}{L}\right)}{2M}\sec^2\left(\frac{\pi\mathbf{Q}}{L}\right), \tag{39}$$

which subsequently yields $k_1 = k + \frac{\pi}{L}$ and $E_1 = \hbar^2\left(k + \frac{2\pi}{L}\right)^2/2M$. Continuing in this fashion, I find that $k_n = k + \frac{n\pi}{L}$ and $E_n = \hbar^2\left(k + \frac{n\pi}{L}\right)^2/2M$, for $0 \le n$. One interesting aspect of this solution is that if we choose $k = 0$ for the initial potential, then it corresponds to the solution of the conventional particle-in-a-box problem with the box situated from $x = -\frac{L}{2}$ to $x = \frac{L}{2}$.

One can see that this approach uses just the properties of the matrices in carrying out the calculations, and hence, it would have been a feasible approach for solving additional problems with matrix mechanics. However, it does require the notion of the quantum state, even if we do not use it in the final calculations, and that was not available to Heisenberg, Born, and Jordan until Schrödinger formulated a quantum theory in terms of quantum states.

5 Discussion

Therefore, what do we learn from this exercise? One thing is that perhaps the discoverers of matrix mechanics gave up too soon in their pursuit of developing quantum mechanics from the matrix mechanics approach. Had they recognized how factorization was the key to solving these problems, then they easily could have developed the theory along the lines discussed here. However, because they did not understand how factorization yields a positive semidefinite form, this did not happen until 1940, when Schrödinger discovered how to do it (but with a focus on thinking in terms of the wavefunctions, not the matrices).

Therefore, what was the direction they did try? Their approach focused on finding the matrices for $\mathbf{P}$ and $\mathbf{Q}$ that would yield a diagonal matrix for $\mathbf{H}$. To this day, no one has figured out how to do this for infinite matrices. Of course, it can, and is done routinely in some of the numerical methods used to solve quantum problems, but with a truncated matrix that is a finite size and usually in a basis, where position is diagonal and momentum and the Hamiltonian are not. The finite truncation brings in problems, as we know it must—once the energy eigenvalues are high enough, they become inaccurate, because the truncation affects the results in a significant way.

The best description for how one might have proceeded in a fashion that maps onto modern ideas and requires the solution of a linear problem is given in Section 35 (Chapter 5) of Tomanaga's famous quantum mechanics textbook [16]. There, he describes how one would not try to solve the complicated nonlinear equations, as originally formulated by Heisenberg, but instead, we would pick a concrete basis for the $\mathbf{P}$ and $\mathbf{Q}$ matrices. He chose the harmonic oscillator matrices at time $t = 0$, because they are known concretely. Then, these matrices automatically satisfy the canonical commutation relation and one can use them to calculate the Hamiltonian. Here, one finds that the Hamiltonian matrix is, in general, not diagonal. However, now it can be diagonalized by applying a unitary transformation to transform the momentum and position matrices from the simple harmonic oscillator basis, to the eigenbasis of the problem at hand. Tomanaga couches his discussion in terms of first solving it for a finite-sized system (truncated from infinity) and then discusses the general problem. Of course, he provides no examples of how to precisely find these unitary transformations, as no one knows precisely how to do it. However, from a formal development, his approach is much nicer than the original one by Heisenberg, Born, and Jordan, in that it is now a linear eigenvalue problem that needs to be solved.

In the end, Tomanaga's approach is really just a formal one that cannot be carried out for any nontrivial energy eigenvalue problem. Therefore, one needed to find another way. The factorization method is just such a way to do it, but it cannot be done solely with matrices—it needs the knowledge of states.

6 Conclusions

It is a useful exercise to reconsider the discovery of matrix mechanics as we reach its 100th anniversary. The matrix mechanics approach, while almost a lost art today, illustrates an elegant argument for how to find the energy eigenvalues without having energy eigenstates or wavefunctions. While this original form cannot be generalized to solve other problems, a small tweak of the approach, along the lines of the Schrödinger factorization method, allows us to solve all of the analytically solvable problems using a matrix mechanics methodology. It only requires us to use some *ad hoc* rules about how we construct the factorization to make it work. It is unfortunate that Heisenberg, Born, and Jordan did not see how this could be done and were not able to find additional problems to solve this way.

Many of us might prefer the more conventional differential equation and wavefunction approach. However, it has a certain level of mathematical complexity to it—namely, the need to solve problems using series solutions and to perform an appropriate analysis to show that the eigenstates are normalizable wavefunctions. Furthermore, it teaches an approach that rarely is used in modern day research problems, which focus more on working with operators for the many-body problem and for quantum field theory. This allows us to ask the question, is the wavefunction-based approach really the best way to teach quantum mechanics? Or, can we learn something new about alternative ways to proceed based on a matrix mechanics form of reasoning? It is worthwhile to think through these questions rather than jumping to an answer. I hope the presentation here has stimulated just such thoughts.

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