Comments on Adiabatic Quantum Algorithms

Mary Beth Ruskai

Abstract. Recently a method for adiabatic quantum computation has been proposed and there has been considerable speculation about its efficiency for NP-complete problems. Heuristic arguments in its favor are based on the unproven assumption of an eigenvalue gap. We show that, even without the assumption of an eigenvalue gap, other standard arguments can be used to show that a large class of Hamiltonians proposed for adiabatic quantum computation have unique ground states.

We also discuss some of the issues which arise in trying to analyze the behavior of the eigenvalue gap. In particular, we propose several mechanisms for modifying the final Hamiltonian to perform an adiabatic search with efficiency comparable to that for 3-SAT. We also propose the use of randomly defined final Hamiltonians as a mechanism for analyzing the generic spectral behavior of the interpolating Hamiltonians associated with problems which lack sufficient structure to be amenable to efficient classical algorithms.

1. Introduction

Recently there has been considerable interest in a proposed scheme for adiabatic quantum computation and speculation that it may even provide a mechanism for efficient solution of hard problems. Both the validity of the adiabatic theorem and the arguments for its efficiency depend on the existence of an eigenvalue gap. However, the existence of such a gap has not been proven. It has been conjectured on the basis of numerical simulations and the so-called non-crossing rule.

The adiabatic quantum algorithm is designed to take the ground state of an initial Hamiltonian \( H_0 \) to that of a final Hamiltonian \( H_1 \) using a linear interpolating Hamiltonian of the form \( H(s) = (1-s)H_0 + sH_1 \). The quantum adiabatic theorem can be used to show that the efficiency of the adiabatic approximation is \( O(1/g_{\text{min}}) \) where \( g_{\text{min}} \) denotes the minimum energy gap \( g(s) = E_1(s) - E_0(s) \) between the ground and first excited states of \( H(s) \). Thus the efficiency of adiabatic quantum computation depends on how rapidly the eigenvalue gap decreases.

2000 Mathematics Subject Classification. Primary 81P68; Secondary 81Q99.

Partially supported by the National Security Agency (NSA) and Advanced Research and Development Activity (ARDA) under Army Research Office (ARO) contract number DAAG55-98-1-0374 and by the National Science Foundation under Grant number DMS-0074566.

©2002 by author. Reproduction of this article, in its entirety, is permitted for non-commercial purposes.
as the size of the problem increases. The purpose of this note is not to resolve this question, but to discuss some of the issues that arise.

Farhi, et al \[8, 9\] (hereafter referred to as FGG) typically use an initial Hamiltonian of the form

$$H_0 = \frac{1}{2} \sum_j a_j [\sigma_x(j) + I] \equiv \frac{1}{2} \sum_j a_j I \otimes I \ldots \otimes [\sigma_x + I] \ldots \otimes I$$

(1.1)

with $a_j$ a non-negative integer. The eigenstates of $H_0$ are products of eigenstates of $\sigma_x$. The so-called “computational basis” $|k_1 \ldots k_n\rangle$ consists of products of eigenstates of the Pauli matrix $\sigma_z$. (However, it is customary to identify each $k_i$ with an element of $Z_2 = \{0, 1\}$ rather than with the usual eigenvalues of $\pm 1$ or, equivalently, replacing $\sigma_z$ by $\frac{1}{2}[\sigma_z + I]$ as has been done above.) In the computational basis, the eigenstates of $H_0$ have the form $2^{-n/2} \sum_{k_1 \ldots k_n} \pm 1 |k_1 \ldots k_n\rangle$ (with all signs $+1$ for the ground state). FGG define a non-negative final Hamiltonian $H_1$ which is diagonal in the computational basis and has the solution of some problem as its ground state, e.g., they encode the problem known as “3-SAT” in the computational basis. We note here only that this encoding results in a Hamiltonian of the form

$$H_1 = \sum_{k_1 \ldots k_n} E_{k_1 \ldots k_n} |k_1 \ldots k_n\rangle\langle k_1 \ldots k_n|$$

(1.2)

where the ground state energy is zero and the other $E_{k_1 \ldots k_n}$ are positive integers with an upper bound that is $O(n^3)$.

First, we point out that the non-crossing rule is completely inadequate for the purpose of establishing a gap. There are realistic models of physical systems which do exhibit crossings, despite the absence of a symmetry common to both the initial and final Hamiltonians $H_0$ and $H_1$. The most well-known such system is $H_{2^+}$, the hydrogen molecule ion \[13\]. Another example is the Hubbard model for benzene \[15\]. The non-crossing rule and the limitations on its applicability to adiabatic quantum computation are discussed in Appendix B.

However, the most one could hope to gain from the non-crossing rule is uniqueness of the ground state. Fortunately, a standard argument based on the Perron-Frobenius theorem \[17, 21\] suffices for that purpose. This argument is sketched in the Section 3, but does not address the more fundamental issue of the size of the resulting eigenvalue gap.

Some insight into the issues raised by adiabatic computation can be obtained by considering various strategies for replacing FGG’s final Hamiltonian $H_1$ by a modification whose ground state is the solution of Grover’s search problem. We argue that if their algorithm is sufficiently robust to solve an NP problem in polynomial time $O(N^p)$, then a modification should be able to perform a successful search of an unordered list of $M$ items in $O(\log M/p^p)$ time, violating the conventional wisdom that Grover’s algorithm (which requires $O(\sqrt{M})$ time) is optimal. A model problem suggested by FGG shows that this simplistic expectation need not hold; however, their example also suggests that gaps are associated with the presence of a symmetry, not its absence.

The issues raised here involve questions in several subfields of physics and computer science. In order to make this note accessible to people with diverse backgrounds ranging from Schrödinger operator theory to computer science, two appendices are included — one on Grover’s algorithm and one on the non-crossing rule.
2. Uniqueness of the Ground State

Although proof of an eigenvalue gap is likely to be difficult, proving that systems of the type considered by FGG have a unique ground state is easier. It relies on a standard argument widely used [23] to prove uniqueness (and positivity) of the ground state in a variety of systems, including quantum lattice models. There is no particular originality in the argument given below. We present it only in the hope of clarifying some issues, particularly the distinction between the uniqueness of the ground state and the existence of a lower bound on the size of the resulting eigenvalue gap.

The ground state of the initial Hamiltonian (1.1) is easily seen to be unique and consists of products of ground states of $\sigma_z(k)$. However, we wish to transform $H_0$ to the computational basis of products $|k_1 k_2 \ldots k_n\rangle$ of eigenstates of $\sigma_z(k)$. This is easily achieved using tensor products of the Hadamard transform. Instead of examining $H_0$ itself, we consider the operator $F = e^{-H_0}$. The ground state of $H_0$ is the eigenfunction corresponding to the largest eigenvalue of the matrix

$$F = e^{-H_0} = \bigotimes_{k=1}^{n} e^{-a_k |\sigma_z(k)+1|/2} = B_1 \otimes B_2 \ldots \otimes B_n$$

where

$$B_k = \frac{1}{2} e^{a_k/2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 0 & e^{-a_k/2} \\ e^{a_k/2} & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

(2.2)

Now, since all elements of each $B_k$ are strictly positive, their tensor product $F = e^{-H_0}$ also has strictly positive elements. Hence, by the Perron-Frobenius theorem [17, 21] the largest eigenvalue of $F$, and the ground state of $H_0$, is unique.

We would like to know that the ground state remains unique for a Hamiltonian of the form $H = (1-s)H_0 + sH_1$. For this, it suffices that $H_1$ is diagonal (in the computational basis) and has a unique ground state. By the Lie-Trotter formula

$$e^{-H} = \lim_{m \to \infty} \left( e^{-s/m} H_1 e^{-1-s/m} H_0 \right)^m$$

(2.3)

The effect of the diagonal matrix $e^{-s/m} H_1$ is simply to multiply each row of $e^{-1-s/m} H_0$ by a positive number of the form $e^{-|\lambda_j|/m}$. Hence the product $e^{-s/m} H_1 e^{-1-s/m} H_0$ also has positive elements and so does its $m$-th power. (Moreover, because $e^{-s/m} H_0 \to 1$ as $m \to \infty$, these positive elements do not become zero in the limit.) Thus, one can again apply the Perron-Frobenius theorem to conclude that the largest eigenvalue of $e^{-H}$ is unique and, hence, $H$ has a unique ground state if $0 \leq s < 1$. (The argument breaks down at $s = 1$ because $e^{-1-s/m} H_0 = I$ no longer has strictly positive elements off the diagonal and is completely decomposable.)

Note that, even if $H_1$ has a degenerate ground state, the interpolating Hamiltonian $H = (1-s)H_0 + tH_1$ will still have a unique ground state for all $0 \leq s < 1$; however, the difference between the two lowest eigenvalues must $\to 0$ as $s \to 1$. Thus, uniqueness of the ground state is a very different matter from an eigenvalue gap of minimal size. Indeed, the uniqueness argument above holds for models [8], such as an adiabatic search for which the gap can be shown to decrease exponentially.
In addition to uniqueness, the Perron-Frobenius theorem implies that the ground state has the form \( \sum_k c_k |k_1k_2 \ldots k_n] \) with strictly positive coefficients \( c_k > 0 \) in the computational basis for all \( s \in [0,1) \). In the limit as \( s \to 1 \) all but one of these \( c_k \to 0 \).

3. Adiabatic Search Algorithms

As described in Appendix A, Grover’s \([12, 13, 22]\) algorithm is designed to efficiently locate an unknown but identifiable target via the use of a unitary operator \( G \) which can be written as \( G = e^{i\pi A} \) where

\[
A |k_1 \ldots k_n] = \begin{cases} 
0 & \text{if } (k_1 \ldots k_n) = (t_1 \ldots t_n) \\
|k_1 \ldots k_n] & \text{otherwise}
\end{cases}
\]

One can easily implement an adiabatic search by choosing for the final Hamiltonian \( H_1 \) in the FGG algorithm the Grover generator, \( A \), above. The adiabatic evolution will take the ground state of \( H_0 \), namely, \( |\psi_0] = 2^{-n/2} \sum_{k_1 \ldots k_n} |k_1 \ldots k_n] \) to the ground state of \( H_1 = A \), namely \( |t_1 \ldots t_n] \). However, FGG have shown that this process takes exponential time. The analysis can be simplified \([25]\) by modifying the initial Hamiltonian \( H_0 \) to reduce the analysis to a two-dimensional problem.

The reduction to a two-dimensional problem, which plays a critical role in Grover’s algorithm, is associated with a \((2^n - 1)\)-fold degeneracy in the adiabatic Hamiltonian \( H_1 \) and \( H_0 \). However, this is not at all essential for the success of an adiabatic search. All that is needed is that the ground state of \( H_1 \) be the target state \( |t_1 \ldots t_n] \). This suggests that one try to modify \( H_1 \) so that its ground state is \( |t_1 \ldots t_n] \), but the eigenvalue distribution of its excited states is similar to that of a final Hamiltonian known to have a gap.

Suppose that a problem is known to have an efficient solution encoded in the final Hamiltonian \( H_1 \). Then setting \( H_2 = GH_1 \), yields a Hamiltonian identical to \( H_1 \) except that the eigenvalue associated with the target state \( |t_1 \ldots t_n] \) is multiplied by \(-1\). (Because \( G \) and \( H_1 \) are both diagonal in the computational basis, they commute and \( H_2 \) is self-adjoint.) Because \( H_1 \) was defined to be non-negative, \( H_2 \) has exactly one negative eigenvalue so that its ground state is now the target state \( |t_1 \ldots t_n] \). Applying the adiabatic algorithm to the modified interpolating Hamiltonian \( H_2(s) = (1-s)H_0 + sH_2 \) should take the ground state of \( H_0 \) to the target state. Moreover, the only effect on the final Hamiltonian is to move one excited state below the previous ground state, without decreasing the final energy gap \( g(1) \). A similar Hamiltonian which is non-negative could be constructed the replacement

\[ E_{k_1 \ldots k_n} \to 0 \quad \text{if } k_1 \ldots k_n = t_1 \ldots t_n \]
\[ E_{k_1 \ldots k_n} \to E_{k_1 \ldots k_n} + 1 \quad \text{otherwise} \]

in \((3.2)\). In either case, one would not generally expect these modifications to significantly affect \( g_{\min}(s) \), in which case the adiabatic search would be as efficient as the solution of the problem encoded in \( H_1 \).

Thus, if Farhi, et al’s projection of an efficiency of \( O(n^p) \) is correct for the problem encoded in \( H_1 \), then one would expect an efficiency of \( O(\log N)^p \) for the adiabatic search of a list of \( N = 2^n \) items described above. However, this would imply that a quantum computer could search an unordered list in time \( O(\log N)^2 \), contradicting the conventional wisdom that a speed-up greater than \( O(\sqrt{N}) \) is not possible \([3, 4, 24, 26]\). This does not necessarily imply a contradiction. The
proofs that $O(\sqrt{N})$ is optimal depend on assumptions about the nature of the
"oracle query" used in the search. However, van Dam, Mosca and Vazirani \[25\] have observed that the encoding of solutions of other problems, such as 3-SAT, in $H_1$ implicitly assume the ability of the computer to perform more general queries. Thus, standard complexity query arguments can not rule out the possibility of polynomial time algorithms.

After seeing a preliminary version of this manuscript, FGG \[10\] pointed out
that the change from $H_1$ to $H_2$ described above can have a dramatic effect on the gap. We describe their example in the next section.

It should also be noted that our expectation that the change from $H_1$ to $H_2$ will not decrease the minimum gap is not based on the presumption that one is a small perturbation of the other. On the contrary, (as FGG \[10\] emphasized) the two Hamiltonians differ by a multiple of a projection, which can have a significant effect on the spectrum. Indeed, it is essential to our strategy to effect such a change in the final Hamiltonian. However, unless this also induces a change in the structure of the problem, such as a symmetry-breaking, this need not affect the generic behavior of the spectra of the interpolating Hamiltonian; in particular, it need not lead to an avoided crossing of the two lowest levels.

4. A Separable Model

Let $H_1 = \frac{1}{2} \sum_j [\sigma_z(j) + I]$ and set $a_j = 1$ in $H_0$. Then the interpolating Hamiltonian becomes

\[
H(s) = H_0 + s(H_1 - H_0) = \frac{1}{2} \sum_j \left[ (1 - s)\sigma_x(j) + s\sigma_z(j) + I \right]
\]

This system is separable, and exactly solvable. Since $[(1 - s)\sigma_x(j) + s\sigma_z(j) + I]$ has eigenvalues $\frac{1}{2} (1 \pm \sqrt{1 - 2s + 2s^2})$, the ground state of $H(s)$ has energy $\frac{1}{2} (1 - \sqrt{1 - 2s + 2s^2})$ and the gap $g(s) = \sqrt{1 - 2s + 2s^2}$ is independent of $n$ with $g_{\text{min}} = \frac{1}{\sqrt{2}}$. The system also has a high level of symmetry, since $H(s)$ commutes with elements of the symmetric group $S_n$. In fact, there is an additional accidental degeneracy so that the $(k + 1)$-st eigenvalue is $k$ with a degeneracy of $\binom{n}{k}$ for $k = 0, 1, 2 \ldots n$.

Now if $H_1$ is replaced by $H_2 = GH_1$, the symmetry is broken. However, there is still some symmetry and a high level of degeneracy. Essentially, only one state from each of the $(n + 1)$ non-degenerate levels is affected and the problem reduces to an $(n + 1)$-dimensional one which can be analyzed explicitly and shown to have an exponentially decreasing gap. In effect, an eigenvalue can be associated with the target state and must “cross” the levels lying below it to reach the bottom of the spectrum when $s = 1$. (A more detailed examination shows that the levels become exponentially close and then bounce away with the target information transmitted to the lower level).

Although this shows that the argument sketched in Section 3 above cannot be made rigorous, this model is not generic. The exponentially decreasing gap is the result of a symmetry breaking which should not occur when the Hamiltonian $H_1$ has no symmetry to begin with.
5. Discussion

Farhi, et al.\[8\] analyze several other models for which the gap behavior can be calculated explicitly and shown to decrease slowly (i.e., polynomial in \(n\)). However, as they point out, these models all have a high level of symmetry or structure which would lead to efficient classical algorithms. In some cases symmetry allows a high level of degeneracy which permits one to squeeze \(2^n\) states into \([0, O(n^p)]\) without forcing an exponentially decreasing gap.

In adiabatic computation the typical choices for initial and final Hamiltonians have spectra with high degeneracies and consist of positive integers in a range that is polynomial in \(n\). In general, the interpolating Hamiltonian \(H(s)\) breaks these degeneracies and must squeeze \(2^n\) distinct eigenvalues into a range of the form \([0, O(n^p)]\). Thus, most of them must be exponentially close.

It seem that a polynomial gap is more likely to be associated with the presence of symmetry, which allows high degeneracies, than with its absence.

For excited states, it is irrelevant whether or not the observed mergings are “avoided crossings” or true crossings. The simultaneous coalescence of a large number of excited states is essential to the algorithm. The states of the initial and final Hamiltonians are both product states, those of the initial Hamiltonian are products of eigenstates of \(\sigma_x\), while those of the final Hamiltonian are products of eigenstates of \(\sigma_z\) (and thus elements of the so-called “computational” basis). Therefore, the final ground state is always an evenly weighted superposition of all eigenstates of the initial Hamiltonian. Unlike standard applications of the adiabatic theorem, in which the main contribution comes from a few low-lying states, all of the excited states must contribute to the first-order correction. To do this, these higher excited states must get close in some sense. Fortunately, a quantum computer can make this first order correction efficiently, mixing in all \(2^n\) excited states, and this is where the method gets its potential power. However, in order that low order perturbation theory suffice, it is essential that the gap between the ground and first excited state not decrease too rapidly as \(n\) increases.

The non-crossing rule, which is discussed in Appendix B, is based on the belief that “accidents” are extremely rare so that such phenomena as persistent degeneracy, or level crossings do not occur without some underlying physical phenomenon (such as a symmetry) with implications for the associated mathematical model. This viewpoint would suggest that if the lowest gap is to decrease only polynomially when the other eigenvalues are getting exponentially close, there must be some physical mechanism keeping them apart. We are skeptical that such a mechanism can be found for Hamiltonians which encode the solution of problems which do not have enough structure to yield efficient classical solutions.

This raises another question. Is the spectrum of the interpolating Hamiltonian sensitive to the association of particular eigenvalues with particular eigenstates in the final Hamiltonian, or is it primarily dependent on the eigenvalue distribution? For Hamiltonians with a good deal of structure, the first situation clearly holds, and FGG have observed \[8, 11\] that the behavior of the eigenvalue gap can depend critically on the choice of initial Hamiltonian. However, one expects Hamiltonians which encode solutions to typical instances of classically intractable problems, to lack the structure needed for this sensitivity.

Because of the difficulty in analyzing the behavior of the gap in problems without structure, it may be worth considering a randomly defined Hamiltonian, i.e.,
let the energy in (1.2) have the form $E_{k_1 \ldots k_n} = f(k_1 \ldots k_n)$ where $f$ is a suitable random process. One can then ask if there is a sense in which the eigenvalue gap is “almost always” exponentially decreasing. If so, this would suggest that an exponentially small gap is generic, and likely to occur for NP-complete problems. There is already an extensive literature \cite{j, k, l, m, n} on the spectral behavior of random Schrödinger operators, in which one obtains results about typical Hamiltonians with certain properties rather than one with a fixed potential. Although the model Hamiltonians used here have quite a different structure, and may require the development of new techniques, this approach seems worth considering.

Indeed, one could even define the final Hamiltonian for an adiabatic search by letting $f$ be a random variable taking integer values in $[1, n]$ and choosing

$$
E_{k_1 \ldots k_n} = 0 \quad \text{if } k_1 \ldots k_n = t_1 \ldots t_n
$$

$$
E_{k_1 \ldots k_n} = f(k_1 \ldots k_n) \quad \text{otherwise}
$$

in (1.3).

Acknowledgment: This note is based on a talk at the Q-Math8 conference in Mexico in December, 2001. It is a pleasure to thank the organizers for the opportunity to present these ideas to an audience of mathematical physicists in a delightful setting; to acknowledge helpful discussions with Professors Charles Bennett, George Hagedorn, Chris King, John Preskill, Barry Simon, and Umesh Vazirani; and to thank Professors Edward Farhi and Sam Gutman for suggesting the model in Section 4. Part of this work was done when the author was visiting the Institute for Theoretical Physics at the University of California, Santa Barbara and thereby also partly supported by the National Science Foundation under Grant PHY-9907949.

Appendix A. Grover’s Algorithm

Grover’s \cite{12, 22} algorithm is designed to efficiently locate an unknown but identifiable target state $|t_1 \ldots t_n\rangle$. This state may be the key denoting the location of an item in an unsorted list (e.g., the analogue of the name in an alphabetized phone book associated with telephone number one has been given) or a state with a certain verifiable property, e.g., a representation of the factors of a given number or the solution of some NP-complete problem.

Grover showed how to construct a unitary operator $G$ whose effect is simply to multiply the unknown target state $|t_1 \ldots t_n\rangle$ by $-1$ and all others by $+1$. This operator can then be used to construct an algorithm which will find the target state with probability greater than $\frac{1}{4}$ in $O(\sqrt{N})$, i.e., $O(2^{n/2})$ time for $N = 2^n$ states. The operator $G$ is a unitary operator whose action on the computational basis is simply

$$
G|k_1 \ldots k_n\rangle = \begin{cases} 
-k_1 \ldots k_n & \text{if } (k_1 \ldots k_n) = (t_1 \ldots t_n) \\
|k_1 \ldots k_n\rangle & \text{otherwise}
\end{cases}
$$

It is generally assumed that one has an “oracle” which can perform unitary operations to determine whether or not a state has the desired property and outputs a function $f$ whose value is 1 if the answer is yes and 0 otherwise. This oracle is described by the unitary operator which takes

$$
|k_0\rangle \otimes |k_1 \ldots k_n\rangle \mapsto |k_0 \oplus f(k_1 \ldots k_n)\rangle \otimes |k_1 \ldots k_n\rangle
$$
The action of this oracle when the first bit is in the $\sigma_x$ eigenstate $2^{-1/2}(|0\rangle - |1\rangle)$ (for which we use the somewhat unconventional notation $|1\rangle_x$) is then
\begin{equation}
|1\rangle_x \otimes |k_1 \ldots k_n\rangle \mapsto e^{i\pi f(k)}|1\rangle_x \otimes |k_1 \ldots k_n\rangle
\end{equation}
which is exactly the effect of $G$ when the ancillary initial bit $|1\rangle_x$ is omitted. The power of quantum computing is then exploited by applying $G$ to superpositions of the form $\sum_k c_{k_1 \ldots k_n} |k_1 \ldots k_n\rangle$ rather than to the individual states in the computational basis. The analysis is facilitated by the realization that the problem can be reduced to a two-dimensional one in
\[ \text{span}\left\{ |t_1 \ldots t_n\rangle, \sum_{k_1 \ldots k_n} |k_1 \ldots k_n\rangle \right\} \]
for which $|t_1 \ldots t_n\rangle$ and $\frac{1}{\sqrt{N}}\sum_{k_1 \ldots k_n \neq t_1 \ldots t_n} |k_1 \ldots k_n\rangle$ form an orthonormal basis.

Appendix B. The Non-Crossing Non-Rule

The so-called “non-crossing rule” is one of a number of physical principles which arise when symmetry ensures that a critical term in some expression, such as the leading term in a perturbation expansion, is zero. The remaining conditions needed to obtain a crossing, transition, etc. are then more easily satisfied. In the absence of the canonical conditions, such crossings and transitions are not truly “forbidden”, but are either rare events which result from an accidental confluence or the result of another physical circumstance which facilitates the satisfying of certain conditions.

In the case of interest here, the canonical condition for crossing is that the Hamiltonians $H_1$ and $H_0$ both commute with the operators which generate a symmetry group $G$ (for which it is not necessary that $H_1$ and $H_0$ commute with each other). The irreducible representations of $G$ can then be used to classify the eigenspaces of $H_1$, $H_0$, and the interpolating Hamiltonian $H(s) = (1-s)H_1 + sH_0$. The non-crossing rule asserts that one expects eigenvalues of $H(s)$ to cross only if they belong to different irreducible representations.

A similar situation arises in the Born-Oppenheimer approximation for the hydrogen molecule ion $H_2^+$ in which case the role of $t$ is replaced by the internuclear distance $R$. Standard tables of atomic data, show many instances of crossings of states in the same symmetry class, in apparent violation of the non-crossing rule. In this case, the paradox was rather easily resolved by the discovery of a “hidden symmetry” which can regarded as a generalization of that responsible for the well-known “accidental” degeneracies of states of different angular momentum (but same principle quantum number $n$) for hydrogen. However, the generator of this symmetry group is an operator (denoted $F(R)$ by Judd [18]) which depends on the internuclear distance $R$. Although this gives a satisfactory physical explanation for the phenomena observed, it points out a difficulty with any attempt to make a mathematically precise theorem out of the “non-crossing rule”. If a crossing exists, the degeneracy in $H(s)$ always allows the formal construction of a suitable symmetry group [16].

A less well-known example of violation of the non-crossing rule occurs in Heilmann and Lieb’s study [15] of the Hubbard model for benzene. Moreover, in this case, a rather detailed analysis [16] failed to locate a hidden symmetry, even one dependent on a parameter. In addition, their work found persistent degeneracies
unexplained by symmetry. This is more serious, as it is far less likely to be an artifact of the numerical methods used. It is worth quoting part of their discussion.

The [non-crossing rule] depends crucially on the interpretation of the word symmetry. The conventional meaning is that of a symmetry group independent of [a parameter] \( U \); in this case the “proofs” are false. . . . If one allows symmetry groups that are \( U \)-dependent, the “theorems” are mere tautologies, because . . . one can always invent, \textit{post hoc} a \( U \)-dependent group to account for any violations.

One may ask what is wrong with the “proofs” quoted above. The fault lies not in the mathematics \textit{per se} but in the assumptions used to connect the mathematics with the real world: First, in the natural sciences, two real numbers are never equal unless there is a physical reason for it; second, that reason must be the existence of a \( U \)-independent symmetry group.

The first assumption has validity, but the second is merely a confession of ignorance ...

Although the relevance of the non-crossing rule to adiabatic quantum computation is questionable, the principles underlying it are not. If polynomially decreasing gaps are generic for systems in which exponentially many eigenvalues are squeezed into an interval that increases only polynomially, there must be a physical reason for this behavior.

References

[1] M. Aizenman and S. Molchanov “Localization at Large Disorder and at Extreme Energies: An Elementary Derivation” \textit{Commun. Math. Phys.} \textbf{157}, 245–277 (1993).
[2] M. Aizenman and B. Simon “Brownian Motion and Harnack Inequality for Schrödinger Operators” \textit{Commun. Pure Appl. Math.} \textbf{bf XXXV}, 209–273 (1982).
[3] C.H. Bennett, E. Bernstein, G. Brassard and U. Vazirani “Strengths and Weaknesses of Quantum Computing” \textit{SIAM J. Comput.} \textbf{26}(5), 1510–1523 (1997).
[4] M. Boyer, G. Brassard, P. Hoyer, and A. Tapp, “Tight Bounds on Quantum Searching” \textit{Fortsch. Phys.} \textbf{46} 493–506 (1998).
[5] R. Carmona and J. Lacroix, \textit{Spectral Theory of Random Schrödinger Operators} (Birkhauser, 1990).
[6] A.M. Childs, E. Farhi, and J. Preskill “Robustness of Adiabatic Quantum Computation” \textit{quant-ph/0108068}.
[7] H. Cycon, R. Froese, W. Kirsch and B. Simon \textit{Schrödinger Operators with Application to Quantum Mechanics and Global Geometry} (Springer Verlag, 1987).
[8] E. Farhi, J. Goldstone, S. Gutmann and M. Spiser “Quantum Computation by Adiabatic Evolution” \textit{quant-ph/0001109}.
[9] E. Farhi, et al “A Quantum Adiabatic Evolution Algorithm Applied to Random Instances of an NP-complete Problem” \textit{Science} \textbf{292}, 472–474 (2001); see also \textit{quant-ph/0104129}.
[10] E. Farhi and S. Gutmann, private communication.
[11] E. Farhi, J. Goldstone, S. Gutmann “Quantum Adiabatic Evolution Algorithms versus Simulated Annealing” \textit{quant-ph/0201031}.
[12] L. Grover, \textit{Proceedings 28th Annual ACM Symposium on the Theory of Computing} pp. 212–219 (ACM Press, 1996).
[13] L. Grover, “From Schrödinger’s Equation to the Quantum Search Algorithm” \textit{Am. J. Phys.} 769–777 (2001). \textit{quant-ph/0106114}.
[14] G. Hagedorn and A. Joye, “Elementary Exponential Error Estimates for the Adiabatic Approximation” \textit{J. Math. Anal. Appl.} \textbf{267}, 235–246 (2002).
[15] O. Heilman and E.H. Lieb, “Violation of the Noncrossing Rule: The Hubbard Hamiltonian for Benzene” \textit{Trans. N.Y. Acad. Sci.} Series II \textbf{33}, 116–149 (1971).
[16] O. Heilman, J. Math. Phys. 11, 3317–3321 (1970).

[17] R.A. Horn and C.R. Johnson, Matrix Analysis (Cambridge University Press, 1985).

[18] B.R. Judd, Angular Momentum for Diatomic Molecules (academic Press, 1975).

[19] T. Kato “On the Adiabatic Theorem of Quantum Mechanics” J. Phys. Soc. Jap. 5, 435–439 (1951).

[20] L. Landau and L. Lifshitz, Quantum Mechanics (Second edition of English translation, Pergamon Press, 1965).

[21] M. Marcus and H. Minc, A Survey of Matrix Theory and Matrix Inequalities (Allyn and Bacon, 1964).

[22] M.A. Nielsen and I.L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, 2000).

[23] M. Reed and B. Simon, Methods of Modern Mathematical Physics 4 : Analysis of Operators (Academic Press, 1978).

[24] W. Thirring, Quantum Mechanics of Atoms and Molecules (Springer-Verlag, 1979).

[25] W. van Dam, M. Mosca, U. Vazirani, “How Powerful is Adiabatic Quantum Computation” Proceedings of the 42nd Annual Symposium on Foundations of Computer Science, pp. 279-287 (2001). quant-ph/0206003.

[26] C. Zalka “Grover’s Quantum Searching Algorithm is Optimal” Phys. Rev. A 60, 2746–2750 (1999).

Department of Mathematics, University of Massachusetts Lowell, Lowell, MA 01854 USA

E-mail address: MaryBeth_Ruskai@uml.edu