

# The Computer as a Physical System: A Microscopic Quantum Mechanical Hamiltonian Model of Computers as Represented by Turing Machines

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*Received June 11, 1979; revised August 9, 1979*

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In this paper a microscopic quantum mechanical model of computers as represented by Turing machines is constructed. It is shown that for each number  $N$  and Turing machine  $Q$  there exists a Hamiltonian  $H_N^Q$  and a class of appropriate initial states such that if  $\Psi_Q^N(0)$  is such an initial state, then  $\Psi_Q^N(t) = \exp(-iH_N^Q t) \Psi_Q^N(0)$  correctly describes at times  $t_3, t_6, \dots, t_{3N}$  model states that correspond to the completion of the first, second, ...,  $N$ th computation step of  $Q$ . The model parameters can be adjusted so that for an arbitrary time interval  $\Delta$  around  $t_3, t_6, \dots, t_{3N}$ , the "machine" part of  $\Psi_Q^N(t)$  is stationary.

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**KEY WORDS:** Computer as a physical system; microscopic Hamiltonian models of computers; Schrödinger equation description of Turing machines; Coleman model approximation; closed conservative system; quantum spin lattices.

## 1. INTRODUCTION

There are many reasons to attempt the construction of a quantum mechanical model of computers and the computation process. Computers are large, finite physical systems which play an important role in science today. The success in developing simple quantum mechanical models of complex systems such as lattice systems, ring models,<sup>(1-3)</sup> and the measurement process<sup>(4-6)</sup> encourages one to try to develop such models for these more complex processes.

Of potentially greater importance is the fact that if one is to make any progress toward giving a quantum mechanical description of intelligent beings—if it is possible at all<sup>(7,8)</sup>—then one must first give such a description

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of computers and the computation process. In particular, the computation process consists of a sequence of elementary decision procedures in which the operation carried out in the  $(n + 1)$ th step depends on the results obtained from the operation done in the  $n$ th step. To construct a quantum mechanical model of the computation process means that one can construct a quantum mechanical model of at least simple decision procedures. A priori it is not clear that this is possible.

A further question arises regarding the possibility of constructing a model of the computation process which is not only quantum mechanical but is a Hamiltonian model. Success in this would mean that it is possible to model the computer as an evolving closed, conservative system in quantum mechanics. There are several reasons for thinking that this might not be possible. All computers built so far are open dissipative systems requiring an energy input to run. Also, complex organized systems, which are much discussed,<sup>(9)</sup> are regarded as open dissipative systems which require energy input to maintain their complexity.

Another source of doubt arises from work done on fundamental limitations of the computation process itself. Some of this work<sup>(10-13)</sup> makes the point that computation steps must often erase information and are thus logically (and physically) irreversible. As a result an energy dissipation of the order of  $kT$  per bit erased is required. On the other hand, a computer can always be made logically reversible by having it create and save a history of its computation.<sup>(14)</sup> Also, the existence of logically reversible computers (as Turing machines) which are equivalent to the usual ones and which erase their own history tapes has been demonstrated.<sup>(14)</sup> It is assumed, however,<sup>(14)</sup> that these reversible machines can be modeled by thermodynamically reversible systems which dissipate arbitrarily little energy per step if operated sufficiently slowly. Other types<sup>(13)</sup> of models also require that the computer lose energy in each step, where the energy loss can be made arbitrarily small if the computation proceeds sufficiently slowly.

Another point takes cognizance of the fact that, as already noted, steps of a computation process are decision procedures. It is suggested<sup>(15)</sup> that since the computer acts on the basis of information read or measured in a short time, the Heisenberg uncertainty principle limits the information processing rate of the computer.

These considerations suggest that it may be impossible even in principle to construct a quantum mechanical Hamiltonian model of the computation process. The reason is that any such model evolves as an isolated system with a constant total energy. The point of this paper is to suggest, by construction of such models, that this may not be the case.

The construction of quantum mechanical models of the computation process which are completely satisfactory in all respects is a large undertaking. Thus it is appropriate to proceed in stages by first making some simplifying

approximations and assumptions. These can (one hopes) be removed in later work.

Here several simplifying approximations are made. First this work will be limited to constructing models of the computation process as represented by Turing machines.<sup>(16,17)</sup> Turing machines have the disadvantage that they are very slow—many steps are needed to carry out simple operations. However, this limitation has the advantage that only one type of model need be considered here, and the model is quite simple. Also, this is in essence no limitation, in that Turing machines are very powerful; any digital computer can be replaced by a Turing machine of equal or greater computing power.

The main approximation made here is that the Coleman model<sup>(6,18)</sup> is used for the kinetic energy part of the Hamiltonian. In this model the kinetic energy operator  $\nabla^2/2m$  is replaced by  $v \cdot \nabla$ , where  $v$  is a fixed velocity. This has the consequence that all systems move with constant velocity, energy is proportional to momentum, and there is no wave packet spreading.

This approximation is made here in the same spirit as was done by Bell<sup>(6)</sup> and Hepp.<sup>(18)</sup> It greatly simplifies the mathematical analysis while leaving intact the essential quantum mechanical nature of the process. In particular, the only use made here of the Coleman model is to turn on and off, over and over again, three separate parts of the interaction Hamiltonian which correspond to three types of model steps. This is done by having a sequence of particles move past a fixed system and interact with it by means of a short-range potential. However, all the complexity of the process resides in the interaction Hamiltonian, which is independent of the Coleman model approximation.

Another approximation that will be made is that the model will be restricted to contain a finite number of degrees of freedom. This approximation is made here to avoid for this first stage possible mathematical problems associated with the quantum mechanics of systems with an infinite number of degrees of freedom. This approximation means that the models of Turing machines constructed here will contain tapes of finite length and that they will correctly describe a finite number of steps of a computation process. The usual Turing machine models contain one or more tapes of infinite length and correctly describe all computation processes of a finite or infinite number of steps. On the other hand, all real computers are systems with a finite number of degrees of freedom. In this sense the above restriction is not a restriction, as it correctly represents the real situation. Also, it has been pointed out<sup>(17)</sup> that Turing machines require infinite tapes only in the limit of an infinite number of steps.

Finally one notes that the models of the computation process constructed here all create and save a history tape. Thus the possibility of constructing a quantum mechanical Hamiltonian model of a computation process which erases its own history tape remains an open question.

The organization of this paper is as follows: The relevant material on Turing machines is reviewed in Section 2. In Section 3 the component systems and transformation operators that are needed are assembled. Also, the method of treating elementary decision procedures and the necessity of adding record tapes is discussed.

Section 4 discusses the model calculation procedure as a sequence of three steps—record, operate, and shift—repeated over and over. The interaction Hamiltonians for the three steps are also given and their properties are discussed. These Hamiltonians can be used to give a time-dependent Hamiltonian description of the process. However, a time-independent Hamiltonian is desired. This is obtained by extending the model to include control systems which interact with the machine. The final Hamiltonians and model are given in Section 5, as is the main result noted earlier.

The proof of the main result, which is given as a theorem, is given in the Appendix. Properties of the evolving model state are also given in Section 5. Section 6 contains a discussion of some further aspects of the model.

Finally, it should be noted that, as far as the uses made so far of computers are concerned, it probably<sup>(19)</sup> makes no difference whether a computer is described classically or quantum mechanically. However, there is an area of questions which is largely unexplored, where the description used may have an effect.

Consider, for example, the fact that one tests the validity of quantum mechanics by carrying out repetitions of an experiment and comparing the limit mean so obtained with a theoretical expectation value calculated on a computer. If the machine used to compute the expectation value is described by the same theory (QM) whose validity is being tested, interesting self-consistency questions can arise. These questions are meaningless if the computer is described by a theory (CM) which is different from that whose validity is being tested.

## 2. TURING MACHINES

A Turing machine<sup>(16,17)</sup> consists of a machine and an infinite tape divided into cells. Each cell of the tape may be blank or it may contain one of a finite number of symbols. The finite symbol string present on the tape at any time is called the tape expression. The machine scans one tape cell at a time and can either change the tape symbol or print one if the cell is blank, or shift one cell to the right, or one cell to the left, or do nothing. The machine can assume any one of a finite number of states called “internal states.”

An elementary Turing machine operation consists of the machine in an internal state carrying out one of the above operations on the tape cell it is scanning and then going to some other internal state. The operations are represented by elementary quadruples of the form  $a(t, t')b$ , where  $a$  and  $b$

denote the initial and final internal machine states,  $t$  denotes the symbol scanned, and  $t'$  denotes either a symbol or an operation  $R$  (shift one cell to the right) or  $L$  (shift one cell to the left). From now on the blank denoted by  $b$ , is considered as a symbol. For example, the quadruple  $a_i(ss')a_m$  means that the machine in internal state  $a_i$  in scanning a cell first reads the cell symbol. If it sees  $s$ , it changes the symbol to  $s'$  and then its internal state changes to  $a_m$ . The quadruple  $a_i(bR)a_k$  means that the machine in internal state  $a_i$  shifts one cell to the right if the cell scanned is blank. Then it goes into internal state  $a_k$ .

In order to present machines by sets of quadruples it is necessary to adhere to certain conventions. A standard initial state of a calculation is represented by the machine being in a designated initial state  $a_i$  and scanning the blank cell immediately to the left of the first nonblank cell. The tape expression is also in a standard form, which means that at most a finite number of cells are nonblank and no two nonblank cells can have a blank cell in between. The standard final state is exactly the same, except that the machine is in a designated final state  $a_f$ .

Turing machines can be represented by finite sets of quadruples. In such a representation the successive steps in a calculation are determined by the quadruples in the set. If the machine, after completing a step, is in internal state  $a_m$ , the next step is determined by that quadruple beginning with  $a_m$  and whose second symbol is the symbol in the tape cell being scanned. For a calculation to be uniquely determined by a set of quadruples it is necessary and sufficient that no two quadruples have the same first two symbols—such a set is called *deterministic*. A calculation terminates if the machine has arrived in internal state  $a_m$  and is scanning a cell containing the symbol  $s$  and no quadruple in the set begins with  $a_m$  and  $s$ . A calculation is nonterminating if the set of quadruples is such that each step in the calculation always has a next step. Whether a particular calculation will terminate or not depends both on the set of quadruples and on the initial tape expression.

The above can be collected together into the following: Every standard Turing machine can be represented by a finite deterministic set  $Q$  of quadruples such that at least one quadruple begins with  $a_i$  and at least one ends with  $a_f$  and no quadruples end with  $a_i$  or begin with  $a_f$ .

From now on we will suppress the distinction between a Turing machine and its representation and will call any  $Q$  that satisfies the above a Turing machine.

Here are two examples of standard Turing machines:

$$Q_1 = \{a_i(b, R)a_1; a_1(b, 1)a_2; a_1(1, 1)a_3; \\ a_3(1, R)a_1; a_2(1, L)a_2; a_2(b, b)a_f\}$$

$$Q_2 = \{a_i(b, R)a_1; a_1(1, 1)a_2; a_2(1, R)a_1; \\ a_1(b, L)a_1; a_1(0, 1)a_3; a_3(1, L)a_3; a_3(b, b)a_f\}$$

The tape symbols for machine  $Q_1$  consist of the blank and the symbol 1. The machine  $Q_1$  calculates the function  $f(n) = n + 1$  by adding a symbol 1 onto a string of 1's before returning to the left of the tape symbol string.  $Q_1$  always terminates. The tape symbols for  $Q_2$  consist of  $b$ , 0, and 1. The machine  $Q_2$  changes the first 0 appearing in the tape expression to a 1 before returning to its initial scanning position.  $Q_2$  may or may not terminate, depending on whether the tape expression contains any 0's or not.

As was noted before, Turing machines are very slow but are very simple and powerful—any digital computer, present or contemplated, can be replaced by (much slower) Turing machines of equal or better computing power. Also, there exist universal Turing machines. A universal Turing machine, when given a code or Gödel number of any Turing machine  $Q$  followed by a symbol expression  $\alpha$  on the input tape, acts like  $Q$  and gives as output the same expression as  $Q$  would, given  $\alpha$  as input. For more details and examples of Turing machines the reader is urged to consult the literature.<sup>(16,17)</sup>

### 3. A QUANTUM MECHANICAL MODEL FOR STANDARD TURING MACHINES

In order to construct a quantum mechanical model it is first necessary to assemble together specific representations for the tape and internal machine states as well as operators which represent the elementary operations of the tape. Much of the construction will be modeled after the various models of the measurement process which have been discussed in the literature.<sup>(4-6,18)</sup>

The final model will be obtained by starting with a simple model and extending it in stages. This is done in order to make quite clear why it is necessary to expand the model by adding auxiliary systems with specified functions. The first simple model consists of a tape  $T$  of finite length divided into cells, a computation head  $H_C$  which moves along the tape and which reads and operates on the symbols in the cells, and a machine  $M$  which is capable of assuming any one of a finite number of internal states. From now on the term "Turing machine" will refer to the system  $M + T + H_C$  plus any other added systems. The term "machine" will refer to  $M$  only.

The tape is represented here by a lattice of quantum spin systems of finite length. The tape alphabet, which is the set of possible symbols, blank included, that can appear in any cell, is assumed to be in one-to-one correspondence with the set of possible spin projections that each of the spin systems is capable of assuming. Thus an expression (as a symbol string) of length  $n$  corresponds to a length- $n$  lattice system in a product state in which the  $j$ th system is in a spin projection eigenstate which corresponds to the  $j$ th symbol of the expression. A spin lattice of length  $n$  is thus suitable for representing all tape expressions

of length  $n$  or less and written in an alphabet of  $2s$  nonblank symbols, where  $s$  is the total spin of each system in the lattice (one of the  $2s + 1$  projections represents the blank).

For reasons which will be clear later, the tape spin lattice is specialized to be of length  $2N + 1$  with the spin systems occupying positions  $-N, \dots, -1, 0, 1, \dots, N$  along the  $x$  axis. The machine system  $M$  corresponds to a single system of spin  $s_Q$  fixed at the lattice position  $x_0$ . The possible internal states that  $M$  can assume are in one-to-one correspondence with the spin projections of the system. Thus for each Turing machine  $Q$ ,  $s_Q$  must be sufficiently large so  $2s_Q + 1$  is greater than or equal to the total number of distinct internal machine states appearing in the quadruples of  $Q$ . Since  $s_Q$  depends on  $Q$ , which system one uses in the model to represent  $M$  depends on  $Q$ .

The computation head  $H_C$  will be represented in the model by a single spinless system which moves along the  $T$  lattice. The quantum states for this system will be taken to be given by the Hilbert space  $l^2([Z_{2N+1}])$ , the space of all sequences  $z: [-N, N] \rightarrow C$  of length  $2N + 1$ . Here  $C$  is the set of complex numbers.

To facilitate the discussion, from now on the distinction between the Turing machine components  $M, T$ , and  $H_C$  and the physical systems which represent them will be, for the most part, suppressed. It will always be clear from the context which is being discussed.

The operators for changing the spin projections, which correspond to the internal machine state change represented by some quadruple  $q$ , are elements of the spin algebra  $\mathfrak{A}_M$ . If  $U_{lm}$  is the spin change operator, which exchanges the spin projections corresponding to the internal states  $a_l$  and  $a_m$  and leaves the others alone, one has

$$\begin{aligned} U_{lm}P_m &= P_lU_{lm} \\ U_{lm}P_l &= P_mU_{lm} \\ U_{lm}P_n &= P_nU_{lm} \quad \text{if } n \neq l, m \end{aligned} \tag{1}$$

where  $P_n$  is a projection operator onto the spin projection corresponding to the machine internal state  $a_n$ . Since  $U_{lm} = U_{lm}^*$ , one has the result that  $U_{lm}$  is self-adjoint and

$$U_{lm}^2 = \mathbf{1} \tag{2}$$

The algebra of operators for the spin lattice that represents the tape  $\mathfrak{A}_T$  is given by

$$\mathfrak{A}_T = \bigotimes_{j=-N}^N \mathfrak{A}_j \tag{3}$$

where  $\mathfrak{A}_j = B(\mathcal{H}_j)$ , the space of bounded linear operators over the  $(2s + 1)$ -dimensional Hilbert space  $\mathcal{H}_j$ .

The operator that exchanges the symbols  $v$  and  $v'$  in cell  $k$  and leaves the other symbols in cell  $k$  alone and does not change symbols in other cells,  $U_{vv'}^k$ , satisfies

$$\begin{aligned} U_{vv'}^k P_{vk} &= P_{v'k} U_{vv'}^k \\ U_{vv'}^k P_{v'k} &= P_{vk} U_{vv'}^k \\ U_{vv'}^k P_{tj} &= P_{tj} U_{vv'}^k \quad \text{if } t \neq v, v' \text{ or } j \neq k \end{aligned} \tag{4}$$

where the projection operators  $P_{tj}$  for the symbol  $t$  in cell  $j$  satisfy

$$\sum_t P_{tj} = 1, \quad P_{tj} P_{t'j} = P_{tj} \delta_{t,t'} \tag{5}$$

for each  $j$ . Note that in general  $P_{tj} P_{t'j'} \neq 0$  if  $j \neq j'$ . As before, one has  $U_{vv'}^k = U_{vv'}^{k\dagger}$  self-adjoint, so

$$(U_{vv'}^k)^2 = 1 \tag{6}$$

Note that in the last paragraph the difference between the tape cell symbols and the corresponding spin projections of a spin system at a lattice site has been suppressed. We shall continue to do this and use machine internal state and tape symbols as parameters for the above operators.

The reason that the symbol and state changing operators are constructed to have the property  $U^2 = 1$  is that, following Bell,<sup>(6)</sup> the fact that

$$e^{\pm iUa} = \cos a \pm iU \sin a \tag{7}$$

will be used to construct the Hamiltonian. In particular, things will be arranged so that the coefficient  $a = a(t) = 0$  for  $0 < t \leq t_j$  and  $0 \leq a(t) \leq \pi/2$  for  $t_j \leq t \leq \tau_j$  and  $a(t) = \pi/2$  for  $t \geq \tau_j$ . Thus  $\exp[-iUa(t)]$  will give, as time progresses, the appropriate change on the system.

The operators that shift the computation head one cell to the left or right are elements of  $B(l^2(Z_{2N+1}))$  and are defined by

$$U_{\pm 1}^k P_j = P_{j'} U_{\pm 1}^k \tag{8}$$

where  $j' = k \pm 1$  if  $j = k$ , and  $j' = k$  if  $j = k \pm 1$ , and  $j' = j$  if  $j \neq k, k \pm 1$ , and  $P_j$  is the projection operator for  $H_C$  being at cell site  $j$ . One also has

$$U_{\pm 1}^{\pm N} P_{-N} = P_N U_{\pm 1}^{\pm N} \quad \text{and} \quad U_{\pm 1}^{\pm N} P_N = P_{-N} U_{\pm 1}^{\pm N} \tag{9}$$

The operator  $U_{+1}^k$  is used to shift  $H_C$  at  $k$  one step to the right and  $U_{-1}^k$  is used to shift  $H_C$  at  $k$  one step to the left. The  $U_{\pm 1}^k$  also have the property given in Eq. (7).

Probably the most important element of the construction is the following: A Turing machine computation is, in essence, a sequence of decision procedures where each operation to be carried out depends on the machine internal state and tape symbol being scanned. Overall this can be regarded as



an operation in which the machine internal state and tape symbol are both read, and the results of the reading determine both the state changing operation and the computation head and tape operation. Machine quadruples express this quite succinctly.

Quantum mechanically, one might consider expressing this as follows: Measure observable  $A = \sum aP_a$  on a system, then, depending on which value  $a$  is found, carry out the operation given by  $U_a$  on the system. The overall operation on the system can be expressed by

$$\sum_a e^{-iB_a P_a}$$

where  $B_a$  is the self-adjoint operator such that  $\exp(-iB_a) = U_a$ , which is supposed to be unitary.

The desired goal of constructing a Hamiltonian is attained in this paper by requiring that the following hold, where  $c$  is an arbitrary constant:

$$\exp\left(-ic \sum_a B_a P_a\right) = \sum_a [\exp(-icB_a)]P_a$$

However, one can show that this equality holds iff  $[P_a, B_{a'}] = 0$  for all  $a$  and  $a'$ . Now  $[P_a, B_{a'}] = 0$  is just what is *not* wanted, since, for the case above, it means that carrying out the  $U_a$  operations has no effect on the system as far as the  $A$  measurement values are concerned.

The solution to this problem which is used here is as follows: First measure  $A$  and transfer the results to a separate record system. Then read the record system and, depending on what is read, carry out the corresponding operation on the original system. The first step can be described by the description of the measuring process given by Von Neumann<sup>(4)</sup> in which a correlation between system eigenstates and apparatus record states evolves by the action of a suitable Hamiltonian.

In this case the second step is expressed by  $\sum_a \exp[-icB_a \otimes 1] 1 \otimes P_a^R$ . However, here one does have

$$\exp\left(-ic \sum_a B_a \otimes P_a^R\right) = \sum_a \exp(-icB_a \otimes 1^R) 1 \otimes P_a^R \quad (10)$$

since  $[B_a \otimes 1, 1 \otimes P_a^R] = 0$  for all  $a, a'$  ( $P_a^R$  is the projection operator for the record system having outcome  $a$  recorded). Equation (10) thus holds even if for the eigenprojectors  $P_a$  of  $A$ ,  $[P_a, B_{a'}] \neq 0$ .

In order to apply this to the quantum mechanical model being constructed it is necessary to extend the system by adding recording systems. For our purposes it is necessary to add a recording head  $H_R$  and at least one record

tape.<sup>3</sup> However, for ease and clarity of exposition, three record tapes, as three quantum spin lattices, will be added. The reason is that it is necessary to record, for each calculation step, the machine internal state, the symbol in the cell being scanned, and the position of the computation head. The reason why these three are needed will become clear later.

Thus three quantum spin lattices  $R_M$ ,  $R_C$ , and  $R_P$  with their associated spin algebras  $\mathfrak{A}_{R_M}$ ,  $\mathfrak{A}_{R_C}$ , and  $\mathfrak{A}_{R_P}$  are added. The subscripts  $R_M$ ,  $R_C$ , and  $R_P$  stand for record machine, record computation, and record position, respectively. The algebras all have the same product structure as  $\mathfrak{A}_T$ , i.e.,  $\otimes_{j=1}^N \mathfrak{A}_j$ , with  $\mathfrak{A}_j$  a single system spin algebra. The systems in  $R_C$  are exactly the same as in  $T$ , the computation tape spin lattice. However, the spin  $s_M$  of the systems in  $R_M$  must be such that  $2s_M + 1 \geq$  the total number of distinct internal machine states in the quadruples of  $Q$ , and the spin  $s_P$  of the systems in  $R_P$  must be such that  $2s_P + 1 \geq 2N + 1$ . Also, the lattices each have only  $N$  systems instead of  $2N + 1$  as needed for  $\mathfrak{A}_T$ .

Since the initial states of all cells in the record tapes will be blank, the desired recording operators are  $U_{bl}^{Mk'}$ ,  $U_{bv}^{Ck'}$ , and  $U_{bk}^{Pk'}$ , which, in the  $k'$ th cells of the three tapes, exchange a blank for the internal state  $l$ , the computation symbol  $v$ , and the computation head position  $k$ , respectively, and make no other changes. They satisfy equations like those satisfied by the computation tape symbol change operator  $U_{vv'}^k$ , i.e., like Eqs. (4).

The states and observables for the recording head  $H_R$  are described in  $l^2(\mathbb{Z}_N)$  and  $B(l^2(\mathbb{Z}_N))$ , respectively. This Hilbert space and operator algebra are exactly the same as those given for the computation head except that the sequence length is  $N$  instead of  $2N + 1$  as is needed for the computation head and tape.

It is worthwhile to collect together the results obtained so far and explain the different lattice system lengths. The component systems consist of a machine, as a system fixed at position  $x_0$ , and with an internal state spin algebra  $\mathfrak{A}_M$ , a computation tape with cells at positions  $-N, \dots, 0, \dots, N$  described as a quantum spin lattice with algebra  $\mathfrak{A}_T$  given by Eq. (3), and a computation head as a system whose associated algebra is  $B(l^2(\mathbb{Z}_{2N+1}))$ . One also has the record systems, which consist of a recording head  $H_R$  as a physical system with the associated algebra  $\mathfrak{A}_{H_R} = B(l^2(\mathbb{Z}_N))$  and three record tapes  $R_M$ ,  $R_C$ , and  $R_P$ . Each of these is modeled as a quantum spin lattice of length  $N$  and algebras  $\mathfrak{A}_{R_M}$ ,  $\mathfrak{A}_{R_C}$ ,  $\mathfrak{A}_{R_P}$ , which all have the tensor product form  $\otimes_{j=1}^N \mathfrak{A}_j$ , where  $\mathfrak{A}_j = B(\mathcal{H}_s)$ , with  $\mathcal{H}_s$  the  $(2s + 1)$ -dimensional Hilbert space of states associated with a spin system with spin  $s$ . For  $R_M$  the spin of each cell system must be such that  $2s + 1 \geq$  total number of internal machine states in the

<sup>3</sup> Bennett<sup>(14)</sup> has extended Turing machines by adding a record tape on which the history of the calculation is generated. Our construction here is in some ways similar to his.

quadruples of  $Q$ . For  $R_C$  the spin of each cell system must be the same as for the computation tape system, and for  $R_P$  the spin of each cell system must be equal to  $N$ .

The algebra associated with the overall system  $\mathfrak{A}_Q'$  is just the tensor product of the component algebras, or

$$\mathfrak{A}_Q' = \mathfrak{A}_M \otimes \mathfrak{A}_{H_C} \otimes \mathfrak{A}_T \otimes \mathfrak{A}_{H_R} \otimes \mathfrak{A}_{R_M} \otimes \mathfrak{A}_{R_C} \otimes \mathfrak{A}_{R_P} \tag{11}$$

Since each of these algebras is the set of all bounded linear operators over some Hilbert space, one has that

$$\mathfrak{A}_Q' = B(\mathcal{H}_Q') \tag{12}$$

where  $\mathcal{H}_Q'$ , the Hilbert space for the whole system, is given by

$$\mathcal{H}_Q' = \mathcal{H}_M \otimes \mathcal{H}_{H_C} \otimes \mathcal{H}_T \otimes \mathcal{H}_{H_R} \otimes \mathcal{H}_{R_M} \otimes \mathcal{H}_{R_C} \otimes \mathcal{H}_{R_P} \tag{13}$$

Here  $\mathcal{H}_{H_C} = l^2(\mathbb{Z}_{2N+1})$ ,  $\mathcal{H}_{H_R} = l^2(\mathbb{Z}_N)$ ,  $\mathcal{H}_M$  is a finite-dimensional spin space, and  $\mathcal{H}_T$  and  $\mathcal{H}_{R_M}$ ,  $\mathcal{H}_{R_C}$ , and  $\mathcal{H}_{R_P}$  are tensor products of  $2N + 1$  copies and  $N$  copies, respectively, of finite-dimensional spin spaces.

#### 4. CALCULATION PROCEDURE AND STEP HAMILTONIANS

The system will be considered to be started in a standard initial state. This is one in which the machine is in internal state  $a_i$  (or  $i$ ), the computing head  $H_C$  is at position 0, and the computation tape has blanks everywhere except possibly for a string of symbols of length  $\leq N$ , starting at  $N = 1$ , and extending to the right. Such a string constitutes the input data for the calculation. The recording head  $H_R$  is at position 1, the leftmost cell of the record tapes, which go from 1 to  $N$ , and all the cells are blank.

The calculation will proceed by means of an interaction which first reads the machine internal state  $i$ , the computation tape symbol at the position of the computation head  $b$ , and the position of the computation head 0, and transfers this to the first blank record cells of  $R_M$ ,  $R_C$ , and  $R_P$ . The second step is described by an interaction which reads the first record cells and carries out the corresponding first computation step transformation on the machine, the computation head, and tape spin system. The computation step interaction, which is given by that  $q$  in  $Q$  which begins with  $a_i(b, -)$ , is unique since  $Q$  is deterministic. The third step consists in shifting the record head to the adjacent blank cells.

The calculation will proceed by repeating over and over again the above three steps. It will stop after  $N$  computations when the record head reaches and records into the  $N$ th or rightmost record cells. The reason that  $2N + 1$  tape computation cells with  $N$  on each side of the head  $H_C$  at its initial position are necessary is that how the head moves during the  $N$  calculation

steps depends not only on  $Q$ , which is fixed, but on the input number on the computation tape. Thus  $Q$  could be such that for some input numbers,  $H_C$  is shifted  $N$  steps to the left, whereas for others,  $H_C$  moves  $N$  steps to the right. Thus all possibilities are included by making the tape  $2N + 1$  units long.

It is clear from the above that in the model calculation there are three types of steps: copy, compute, and shift. Thus for each  $N$  and  $Q$  there are three overall system interaction operators  $H_1^{NQ}$ ,  $H_2^{NQ}$ , and  $H_3^{NQ}$  defined as follows:

$$H_1^{NQ} = \sum_{l \in Q} \sum_v \sum_{k=-N}^N \sum_{k'=1}^N (P_l \otimes P_k \otimes P_{v|k} \otimes P_{k'} \otimes U_{bl}^{Mk'} \otimes U_{bv}^{Ck'} \otimes U_{bk'}^{Pk'}) \quad (14)$$

$$H_2^{NQ} = \sum_{q \in Q} \sum_{k=-N}^N \sum_{k'=1}^N (U_q^M \otimes U_{qk}^{H_C T} \otimes P_{k'} \otimes P_{qk'}^M \otimes P_{qk'}^C \otimes P_{kk'}^P) \quad (15)$$

$$H_3^{NQ} = 1 \otimes 1 \otimes 1 \otimes B \otimes 1 \otimes 1 \otimes 1 \quad (16)$$

These operators are given as sums over tensor products of operators in the component spaces for the systems  $M$ ,  $H_C$ ,  $T$ ,  $H_R$ ,  $R_M$ ,  $R_C$ , and  $R_P$  in the order given. The only exception is in Eq. (15), where  $U_{qk}^{H_C T}$  refers to both  $H_C$  and  $T$ .

In Eq. (14) the  $l$  sum is over all machine internal states appearing in the quadruples of  $Q$ , and the  $v$  sum is over all computation tape symbols.  $P_l$ ,  $P_k$ ,  $P_{v|k}$ , and  $P_{k'}$  are projection operators corresponding to finding the machine in internal state  $l$ ,  $H_C$  at position  $k$ , the symbol  $v$  in the computation cell  $k$ , and  $H_R$  at position  $k'$ .

In Eq. (15), which describes the computation step, the  $q$  sum is over all quadruples in  $Q$  and is finite by the definition of a Turing machine.  $U_q^M$  is the machine internal state change given by  $q$ . If  $q$  is  $a_l(-, -)a_m$ , then

$$U_q^M = U_{lm}^M \quad (17)$$

$U_{qk}^{H_C T}$  corresponds to the computation described by  $q$ . If  $q$  is  $-(v, v')-$ , then

$$U_{qk}^{H_C T} = 1 \otimes U_{vv'}^k \quad (18a)$$

If  $q$  is  $-(v, R)-$ , then

$$U_{qk}^{H_C T} = U_{+1}^k \otimes 1 \quad (18b)$$

and if  $q$  is  $-(v, L)-$ , then

$$U_{qk}^{H_C T} = U_{-1}^k \otimes 1 \quad (18c)$$

$P_{qk'}^M$  and  $P_{qk'}^C$  are the projection operators corresponding to the internal machine state and computation symbol, which are the first two symbols in  $q$ , being located in cell  $k'$  of  $R_M$  and  $R_C$ . Thus, if  $q = a_l(v, -)-$ , then

$$P_{qk'}^M = P_{lk'}^M \quad (19a)$$

and

$$P_{qk}^C = P_{vk}^C \quad (19b)$$

In Eq. (16),  $B$  is the self-adjoint operator in  $B(l^2(Z_N))$  such that

$$e^{-iB\pi/2} = U_{+1} \tag{20}$$

where  $U_{+1}$  is the unitary shift operator mod  $N$  on  $l^2(Z_N)$ . That is,

$$U_{+1}P_n = P_{n+1}U_{+1} \tag{21a}$$

for  $n < N$ , and

$$U_{+1}P_N = P_1U_{+1} \tag{21b}$$

All the terms of the  $l, v, k,$  and  $k'$  sums in  $H_1^{Nq}$  are pairwise orthogonal and

$$\sum_l \sum_v \sum_{k'} \sum_k P_l \otimes P_k \otimes P_{vk} \otimes P_{k'} \otimes 1 \otimes 1 \otimes 1 = 1$$

Thus by Eqs. (10), (7), (6) and (4)

$$\begin{aligned} \exp(-iH_1^{Nq}a) &= \sum_{l \in Q} \sum_v \sum_{k=-N}^N \sum_{k'=1}^N \exp[-i(1_{MHCTHR} \otimes U_{bl}^{Mk'} \otimes U_{bv}^{Ck'} \otimes U_{bk'}^{Pk'})a] \\ &\quad \times (P_l \otimes P_k \otimes P_{vk} \otimes P_{k'} \otimes 1_{RMRCRP}) \end{aligned} \tag{22}$$

$$\begin{aligned} &= \sum_{l \in Q} \sum_v \sum_{k=-N}^N \sum_{k'=1}^N (\cos a - i1_{MHCTHR} \otimes U_{bl}^{Mk'} \otimes U_{bv}^{Ck'} \otimes U_{bk'}^{Pk'} \sin a) \\ &\quad \times (P_l \otimes P_b \otimes P_{vk} \otimes P_{k'} \otimes 1_{RMRCRP}) \end{aligned} \tag{23}$$

From this one sees that  $H_1^{Nq}$  is similar to a Hamiltonian which describes the measurement interaction, between  $M \times H_C \times T$  as the system and an  $R_M \times R_C \times R_P$  cell as the instrument, as an evolving correlation between the system and instrument.<sup>(4)</sup> At the time  $a = t = 0$  no correlation exists and the pointers are all blank. At the time  $a = t = \pi/2$  a complete correlation exists. For times  $t > \pi/2$  the correlation decreases and oscillates between complete correlation and no correlation.

$H_2^{Nq}$  has a similar structure to  $H_1^{Nq}$ . It can be seen that the terms in the  $q, k,$  and  $k'$  sums are pairwise orthogonal. In fact the reason the recording head  $H_R$  is present, and the position of the computation head is recorded, is just to secure this orthogonality.

One has, from Eqs. (1), (2), (4), (6), (8), and (9)

$$\begin{aligned} \exp(-iH_2^{Nq}a) &= \sum_{q \in Q} \sum_{k=-N}^N \sum_{k'=1}^N \exp[-i(U_q^M \otimes U_{qk}^{HC'T} \otimes 1_{HRRMRCRP})a] \\ &\quad \times (1_{MHCT} \otimes P_{k'} \otimes P_{qk'}^M \otimes P_{qk'}^C \otimes P_{kk'}^P) + (1 - P_Q) \end{aligned} \tag{24}$$

where

$$P_Q = \sum_{q \in Q} \sum_{k=-N}^N \sum_{k'=1}^N (1_{MHCT} \otimes P_{k'} \otimes P_{qk'}^M \otimes P_{qk'}^C \otimes P_{kk'}^P) \tag{25}$$

The extra term  $1 - P_Q$  is present because  $Q$  can be such that the sums in Eq. (25) do not give  $P_Q = 1$ . For example, not all possible machine internal state-tape symbol combinations need appear as the first two parameters in some  $q$  in  $Q$ . This will be discussed later in connection with the termination of a computation.

As was the case for  $H_1^{N_Q}$  one can, by use of Eqs. (1), (3), (4), (6), (8), and (9), write

$$\begin{aligned} \exp(-iH_1^{N_Q}a) = & \sum_{q \in Q} \sum_{k=-N}^N \sum_{k'=1}^N [\cos a - i(U_q^M \otimes U_{qk}^{H_{CT}} \otimes 1_{H_R R_M R_C R_P}) \sin a] \\ & \times (1_{M H_{CT}} \otimes P_{k'} \otimes P_{qk'}^M \otimes P_{qk'}^C \otimes P_{kk'}^P) + 1 - P_Q \end{aligned} \quad (26)$$

Again one sees that as the time  $a = t$  evolves from 0, each  $q$  calculation begins and is complete at time  $t = \pi/2$ . As  $t$  increases beyond  $\pi/2$ , the calculations are undone.

Equations (20), (24), and (26) show that an appropriate description of the calculation can be given by a time-dependent Hamiltonian  $H_Q(t)$  which becomes  $H_1^Q$ ,  $H_2^Q$ , and  $H_3^Q$  in successive time intervals  $0-\pi/2$ ,  $\pi/2-\pi$ ,  $\pi-3\pi/2$ , etc. More precisely,

$$\begin{aligned} H_1^{N_Q} & & n = 0 \text{ mod } 3 \\ H_N^Q(t) = H_2^{N_Q} & \text{ if } n\pi/2 < t \leq (n+1)\pi/2 \text{ and } n = 1 \text{ mod } 3 \\ H_3^{N_Q} & & n = 2 \text{ mod } 3 \end{aligned} \quad (27)$$

However, the goal here is to construct a model with a time-independent Hamiltonian which successively turns on and off  $H_1^{N_Q}$ ,  $H_2^{N_Q}$ , and  $H_3^{N_Q}$  with a coefficient  $a(t)$  approaching  $\pi/2$  in a finite time and remaining at  $\pi/2$  thereafter. In order to do this the model given so far must be extended to include control systems which pass by the machine one after another and, by interacting with the machine, turn on and off  $H_1^{N_Q}$ ,  $H_2^{N_Q}$ , and  $H_3^{N_Q}$ . The method to be used is essentially that of Bell.<sup>(6)</sup> In what follows the index  $N$  on  $H_i^{N_Q}$  will be suppressed.

### 5. THE MODEL, HAMILTONIAN, AND MAIN RESULT

The final model used here is shown in Fig. 1. A total of  $3N$  control systems pass the machine system located at  $x_0$  and interact with it by means of a finite-range potential. As each system passes the machine system it turns on the appropriate  $H_j^Q$  by an amount equal to the accumulated interaction.  $H_j^Q$  is turned off when the  $j$ th control system is out of range of the machine.

The rest of the system is as before. That is, one has a calculating head, a computation tape, a recording head, and three recording tapes. The scattering between the control systems and  $M$  is assumed to be one-dimensional. The lengths and relative positions of the tapes for the standard initial position are

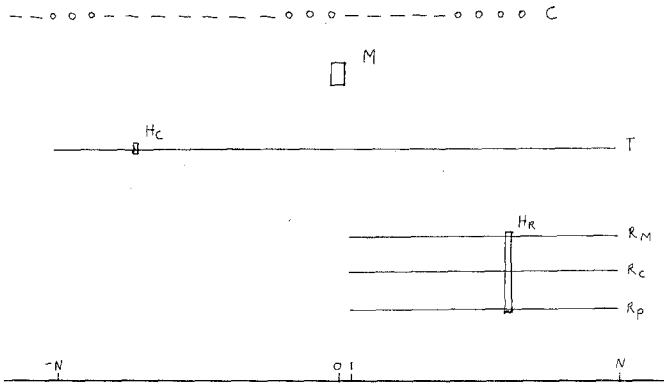


Fig. 1. The final quantum mechanical model. The circles  $C$  represent the  $3N$  control systems. The rectangles  $M$ ,  $H_C$ , and  $H_R$  represent the machine, the computing head, and the recording head, respectively. The lines  $T$ ,  $R_M$ ,  $R_C$ , and  $R_P$  represent the computation tape and the record tapes for recording the machine internal state, the  $T$  symbol scanned, and the position of  $H_C$ . The fixed machine and tape positions are indicated at the bottom.

shown. The heads and control systems represent a possible state of affairs after several calculation steps have occurred. The machine is assumed to be fixed, as on a lattice, at position  $x_0$  which is set equal to zero.

The overall model Hamiltonian for  $N$  steps of machine  $Q$ ,  $H^Q$ , is taken to be

$$H^Q = H_0 + H'^Q \tag{28}$$

where

$$H'^Q = \sum_{j=1}^{3N} V(x_j)H^Q(j) \tag{29a}$$

and

$$H_0 = \sum_{j=1}^{3N} \frac{1}{i} \frac{\partial}{\partial x_j} \tag{29b}$$

In  $H'^Q$ , which is the complete interaction Hamiltonian,  $V(x_j) = V(x_j - x_0)$  gives the interaction potential between the  $j$ th control system and the machine at  $x_0 = 0$ . We define  $H^Q(j)$  by

$$H^Q(j) = \begin{cases} H_1^Q & 1 = j \bmod 3 \\ H_2^Q & \text{if } 2 = j \bmod 3 \\ H_3^Q & 0 = j \bmod 3 \end{cases} \tag{30}$$

where  $H_1^Q$ ,  $H_2^Q$ , and  $H_3^Q$  are given by Eqs. (14)–(16), respectively.

An important simplification has been made for  $H_0$ , the free Hamiltonian, in that the Coleman model has been used<sup>(6,18)</sup> in Eq. (29b). In this model the

particle kinetic energy operator  $\nabla^2/2m$  is replaced by  $v \cdot \nabla$ , where  $v$  is a fixed velocity. All systems move with a fixed velocity, set equal to unity in Eq. (29b), and the kinetic energy is proportional to the momentum.<sup>(6)</sup> This model is used because it makes the mathematics much more tractable—for instance, wave packets evolve without spreading since  $\exp(-iH_0t)$  becomes a displacement operator. This approximation will be discussed further in Section 6.

The interaction Hamiltonian has the feature that the interaction between the parts of the machine depends on the place label  $j$  of the control system. The  $j$ th system turns on  $H^Q(j)$ . This has been done strictly to keep the model simple. If desired, one can slightly improve the model by considering each control system to be a moving, spin-1 system where the  $j$ th system has spin projection  $+1$  if  $j = 1 \pmod 3$ ,  $0$  if  $j = 2 \pmod 3$ , and  $-1$  if  $j = 0 \pmod 3$ , and redefining  $H'^Q$  by

$$H'^Q = \sum_{j=1}^{3N} V(x_j)[P_{+1j} \otimes H_1^Q + P_{0j} \otimes H_2^Q + P_{-1j} \otimes H_3^Q]$$

where  $P_{+1j}$ ,  $P_{0j}$ , and  $P_{-1j}$  are the projection operators for the spin of the  $j$ th control system corresponding to spin projections  $+1$ ,  $0$ , and  $-1$ , respectively.

In what follows  $V(x)$  is assumed to have a finite range. That is,

$$V(x) = 0 \quad \text{if } |x| > r \tag{31}$$

Also, the strength of  $V$  is such that

$$\int_{-\infty}^{\infty} V(x) dx = \int_{-r}^r V(x) dx = \pi/2 \tag{32}$$

The function  $F(y)$ , which is needed later, is defined by

$$F(y) = \int_{-\infty}^y V(x) dx \tag{33}$$

Clearly,  $F(r) = \pi/2$ .

The Hilbert space and operator algebra for the final model,  $\mathcal{H}_Q$  and  $\mathfrak{A}_Q$ , are those given by Eqs. (11)–(13) extended to include the control systems. That is,

$$\mathcal{H}_Q = \mathcal{H}_C \otimes \mathcal{H}'_Q \tag{34}$$

and

$$\mathfrak{A}_Q = \mathfrak{A}_C \otimes \mathfrak{A}'_Q \tag{35}$$

where

$$\mathcal{H}_C = \bigotimes_{j=1}^{3N} L^2(\mathbb{R}_j, dx_j) \tag{36}$$

and

$$\mathfrak{A}_C = B(\mathcal{H}_C) \tag{37}$$



The initial state vector of the system,  $\Psi_Q(0)$ , at time  $t = 0$  will be chosen to represent the initial situation. That is,  $H_C$  at position 0 and  $H_R$  at position 1, the record tapes blank, the only nonblank cells of the computation tape at positions  $> 0$ , no nonblank cells on  $T$  separated by a blank cell, the machine in internal state  $a_i$ , and the control systems all to the left of the machine and out of range. Each control system will be represented by a wave packet  $\varphi$  which has compact support. That is,

$$\varphi(z) = 0 \quad \text{if } |z| > w \tag{38}$$

The overall state at time 0 is given by

$$\Psi_Q(0, x_1, \dots, x_{3N}) = \bigotimes_{j=1}^{3N} \varphi(x_j + d_j) \Psi_Q^{\text{int}}(0) = \Psi^C(0, x_1, \dots, x_{3N}) \Psi_Q^{\text{int}}(0) \tag{39}$$

where

$$\Psi_Q^{\text{int}}(0) = \psi_i^M \otimes \psi_0^{H_C} \otimes \Psi^T \otimes \psi_1^{H_R} \otimes \Psi^R \tag{40}$$

$d_j$  is a spacing parameter which ensures that the  $j$ th particle is localized within  $d_j + w$  and  $d_j - w$ . In what follows  $d_j$  will be set equal to  $jd$ .

Here  $\psi_i^M$  is a pure spin state of the machine internal state spin system, which is an eigenstate of the spin projection operator that corresponds to the initial machine internal state  $a_i$ . The  $\psi_0^{H_C}$  is the state of the computing head localized at 0. That is,  $\psi_0^{H_C} \in l^2(\mathbb{Z}_{2N+1})$  with  $P_0 \psi_0^{H_C} = \psi_0^{H_C}$ . The  $\Psi^T$  is a  $(2N+1)$ -fold tensor product of spin states  $\psi_j^T$  with  $-N \leq j \leq N$ , which correspond to the initial symbols in the tape cells. The  $\psi_1^{H_R} \in l^2(\mathbb{Z}_N)$  localizes the recording head at position 1, and  $\Psi^R = \Psi^{R_M} \otimes \Psi^{R_C} \otimes \Psi^{R_c}$  is the tensor product of the three lattice spin states which correspond to blank symbols in all cells.

The time evolution of  $\Psi_Q(t)$  under the action of  $H_Q$  must now be investigated. The goal is to show that there exist time intervals  $\Delta_1, \dots, \Delta_{3N}$  centered about times  $t_1, \dots, t_{3N}$  such that for each  $j$ , for all  $t \in \Delta_j$ ,  $\Psi_Q(t)$  is in a state which, with probability 1, corresponds to the  $j$ th model step being completed. In fact the following theorem, which is the main result of this paper, can be proved.

**Theorem.** To each standard Turing machine  $Q$  and each  $N$  one can associate a Hamiltonian  $H^Q$  and a class of standard initial states  $\Psi_Q(0)$ , one for each input expression, at time 0, such that if  $d, r$ , and  $w$  satisfy the inequality  $d > 2r + 2w$ , then for times  $t$  such that  $t \leq 3Nd + w + r$ ,  $\Psi_Q(t)$  is given by

$$\begin{aligned} \Psi_Q(t, x_1, \dots, x_{3N}) = & \exp[-iF(x_{n(t)})H^Q(n(t))] \exp[-\frac{1}{2}i\pi H^Q(n(t) - 1)] \\ & \times \dots \exp[-\frac{1}{2}i\pi H^Q(2)] \exp[-\frac{1}{2}i\pi H^Q(1)] \\ & \times \exp(-iH_0 t) \Psi_Q(0, x_1, \dots, x_{3N}) \end{aligned} \tag{41}$$

where  $F(x_{n(t)})$  is given by Eq. (33) and  $n(t)$  is defined to be the smaller of  $3N$  or the largest  $j$  such that  $jd \leq t + w + r$ .

If  $t > 3Nd + w + r$ ,  $\Psi_Q(t)$  is given by

$$\Psi_Q(t, x_1, \dots, x_{3N}) = \exp[-\frac{1}{2}i\pi H^Q(3N) \exp[-\frac{1}{2}i\pi H^Q(3N - 1)] \times \dots \exp[-\frac{1}{2}i\pi H^Q(1)] \exp(-iH_0 t) \Psi_Q(0, x_1, \dots, x_{3N}) \quad (42)$$

The proof of this theorem is given in the Appendix. Here we will discuss it and show that it gives the desired results. The restriction on the control system wave packets and the potential given by  $d > 2r + 2w$  ensures that at each time  $t$  at most one control system is interacting with the machine localized at the lattice point 0. (The machine remains fixed at the lattice point 0 during the interactions with all the control systems.) This can be seen by noting that for the Coleman model used here, Eq. (30),

$$e^{-iH_0 t} \Psi_Q(0, x_1, \dots, x_{3N}) = \bigotimes_{j=1}^{3N} \varphi(x_j + jd - t) \Psi_Q^{\text{int}}(0) \quad (43)$$

Thus the free Hamiltonian shifts the control systems a distance  $t$  to the right. The control system  $j$  interacts with the machine if, for some  $x_j$ ,  $V(x_j)\varphi(x_j + jd - t) \neq 0$ . But this can happen if and only if  $j$  is such that  $t - w - r \leq jd \leq t + w + r$  [Eqs. (31) and (38)]. If  $d > 2w + 2r$ , there is at most one  $j$  for which these two inequalities are satisfied.

We define  $n(t)$  to denote, at any time  $t$ , either the control system that is interacting with the machine or, if none is interacting, the one that has just completed interacting with the machine. As before, the  $j$ th control system is interacting if, for some  $x_j$ ,  $V(x_j)\varphi(x_j + jd - t) \neq 0$ , which happens if and only if  $t - w - r < jd < t + w + r$ . If  $t$  is such that no system is interacting, then the  $j$  value of the one that has just finished is the largest  $j$  such that  $jd < t - w - r$ , which is also the largest  $j$  such that  $jd < t + w + r$ .

Note that the special form of  $\Psi_Q(t)$  given by Eqs. (41) and (42) does not hold in general. It holds only for the restrictions on  $V$ ,  $\varphi$ , and  $d$  noted above. This is quite reasonable even for real computers in that appropriate initial states for a computer plus input system are a small set of all possible states for the overall system.

In order to follow the structure of  $\Psi_Q(t)$  as time increases, it is noted, from Eq. (39) and the structure of  $H^Q$ , that one can commute  $\exp(iH_0 t) \Psi^C(0)$  past all the other factors in Eq. (41) to obtain

$$\begin{aligned} \Psi_Q(t, x_1, \dots, x_{3N}) &= [\exp(-iH_0 t) \Psi^C(0, x_1, \dots, x_{3N})] \\ &\quad \times \exp[-iF(x_{n(t)})H^Q(n(t))] \dots \exp[-\frac{1}{2}i\pi H^Q(1)] \Psi_Q^{\text{int}}(0) \end{aligned} \quad (44)$$

$$= \Psi^C(t, x_1, \dots, x_{3N}) \Psi_Q^{\text{int}}(t) \quad (45)$$

Since

$$\Psi^C(t, x_1, \dots, x_{3N}) = \bigotimes_{j=1}^{3N} \varphi(x_j + jd - t)$$

the computation progress is given by the right-hand factors. From Eqs. (23), (30), and (40) one sees that

$$\begin{aligned} & \exp[-\frac{1}{2}i\pi H^Q(1)] \Psi_Q^{\text{int}}(0) \\ &= -i\psi_i^M \otimes \psi_0^H \otimes P_{b0} \Psi^T \otimes \psi_1^R \otimes U_{bi}^{M1} \Psi^R \otimes U_{bc}^{C1} \Psi^R \otimes U_{b0}^{P1} \Psi^R \end{aligned} \quad (46)$$

where  $P_i \psi_i^M = \psi_i^M \delta_{i,i}$ ,  $P_k \psi_0^H = \psi_0^H \delta_{k,0}$ , and  $P_{k'} \psi_1^R = \psi_1^R \delta_{k',1}$  have been used. Also, the only term in the  $v$  sum that contributes is  $v = b$ , since initially  $H_C$  scans a blank symbol.

Equation (46) gives the state showing the completion of the first copying step. For the next step one has from Eqs. (24) and (25)

$$\begin{aligned} & \exp[-\frac{1}{2}i\pi H^Q(2)] \exp[-\frac{1}{2}i\pi H^Q(1)] \psi_Q^{\text{int}}(0) \\ &= (-i)^2 U_{q_1}^M \psi_i^M \otimes U_{q_1 0}^{HcT} (\psi_0^H \otimes P_{b0} \Psi^T) \otimes \psi_1^R \otimes U_{bi}^{M1} \Psi^R \\ & \quad \otimes U_{bb}^{C1} \Psi^R \otimes U_{b0}^{P1} \Psi^R \end{aligned} \quad (47)$$

where

$$\begin{aligned} P_k \psi_1^R &= \psi_1^R \delta_{k'}, 1, & P_{q_1}^M U_{bi}^{M1} \Psi^R &= U_{bi}^{M1} \Psi^R \delta_{q, q_1} \\ P_{q_1}^C U_{bb}^{C1} \Psi^R &= U_{bb}^{C1} \Psi^R \delta_{q(2), b}, & P_{k_1}^P U_{b0}^{P1} \Psi^R &= U_{b0}^{P1} \Psi^R \delta_{k, 0} \end{aligned}$$

have been used.  $q_i$  denotes any quadruple in  $Q$  beginning with  $a_i$ , and  $q(2)$  denotes the second element of  $q$ , which is always a computation tape symbol. The combination  $\delta_{a_i, q_1} \delta_{q(2), b}$  selects out that  $q$  in  $Q$  whose first symbol is  $a_i$  and whose second symbol is  $b$ —exactly one such  $q$  exists in any standard  $Q$ .

At the completion of the third step one has from Eqs. (16) and (20)

$$\begin{aligned} & \exp[-\frac{1}{2}i\pi H^Q(3)] \exp[-\frac{1}{2}i\pi H^Q(2)] \exp[-\frac{1}{2}i\pi H^Q(1)] \Psi_Q^{\text{int}}(0) \\ &= (-i)^2 U_{q_1}^M \psi_i^M \otimes U_{q_1 0}^{HcT} (\psi_0^H \otimes P_{b0} \Psi^T) \\ & \quad \otimes \psi_2^R \otimes U_{bi}^{M1} \Psi^R \otimes U_{bb}^{C1} \Psi^R \otimes U_{b0}^{P1} \Psi^R \end{aligned} \quad (48)$$

where  $\exp(-\frac{1}{2}i\pi B) \psi_1^R = \psi_2^R$  has been used.

The cycle now begins over again, operating with  $\exp[-\frac{1}{2}i\pi H^Q(4)]$ . This factor and each succeeding factor correspond to the completion of exactly one model step. Operating on the initial state with  $3j$  such factors corresponds to carrying out  $j$  computation steps of the original machine.

For any given time  $t$  one continues as above, evaluating successively from right to left, the effect of the exponential factors until one comes to the last one,  $\exp[-iF(x_{n(t)})H^Q(n(t))]$ . If  $t$  is such that there exist values of  $x_{n(t)}$  such that  $0 < F(x_{n(t)}) < \pi/2$  and  $\varphi(x_{n(t)} + n(t)d - t) \neq 0$  and  $n(t) \bmod 3 = 1$  or  $= 2$ , then by Eqs. (23) and (26), one ends up with a sum over two terms since both  $\cos(F(x_{n(t)}))$  and  $\sin(F(x_{n(t)}))$  are different from zero. This is the case if  $t$  is such that the  $n(t)$ th step is only partly done. This case for  $0 = n(t) \bmod 3$  also gives a linear combination of terms. However, if  $t$  is such that

for all  $x_{n(t)}$  for which  $\varphi(x_{n(t)} + n(t)d - t) \neq 0$ ,  $F(x_{n(t)}) = \pi/2$ , then the  $n(t)$ th factor represents a completed step just as is the case for the other factors.

From this analysis one can see that the parameters can be arranged such that for finite time intervals of width  $\Delta$  centered about  $t_1, t_2, \dots, t_j, \dots, t_{3N}$ , where  $t_j = (j + \frac{1}{2})d$ , the interacting state  $\Psi_Q^{int}(t)$  is stationary for all times in  $\Delta$ . That is, for all times  $t$  such that  $n(t)d + w + r < t < [n(t) + 1]d - w - r$  [which are those times  $t$  such that for all  $x_{n(t)}$  for which  $\varphi(x_{n(t)} + n(t)d - t) \neq 0$ ,  $F(x_{n(t)}) = \pi/2$  and for all  $x_{n(t)+1}$  for which  $\varphi(x_{n(t)+1} + [n(t) + 1]d - t) \neq 0$ ,  $F(x_{n(t)+1}) = 0$ ],  $\Psi_Q^{int}(t)$  is stationary and represents  $n(t)$  completed steps. Thus  $\Delta = d - 2w - 2r$  can be made as large as desired by making  $d$  sufficiently large, with fixed  $w$  and  $r$ .

From the analysis just presented one sees that if the initial state is as given by Eqs. (39) and (40), then at those times for which  $\Psi_Q^{int}(t)$  [Eq. (45)] is stationary,  $\Psi_Q^{int}(t)$  corresponds exactly to the completion of  $n(t)$  model steps. It is not a linear combination over states representing different partially completed or completed steps or over states representing the reading or recording heads in different positions. If  $t$  is such that  $\Psi_Q^{int}(t)$  is not stationary, then  $\Psi_Q^{int}(t)$  is a sum over two or more terms which together represent the partially completed  $n(t)$ th step.

Only if  $\Psi_Q^{int}(0)$  is itself a linear combination of states representing different initial machine internal states, different input tape expressions, and different head positions will  $\Psi_Q^{int}(t)$  be a linear combination of states. However, even in this case the time evolution of  $\Psi_Q^{int}(t)$  preserves the initial linear combination and does not further combine the terms. Speaking diagrammatically, the time evolution of  $\Psi_Q^{int}(t)$  can be represented as a tree in which each path contains no branches, only bubbles, and the only branching is provided initially at the root by the initial state. Of course this all changes if the condition  $d > 2w + 2r$  is relaxed.

It remains to investigate the halting of the computation process. Suppose  $t$  is such that  $\Psi_Q^{int}(t)$  is stationary and  $n(t) = 1 \pmod 3$ . That is, the recording of the tape symbol  $v$ , scanned by  $H_C$ , the position of  $H_C$ , and the machine internal state  $l$  has been completed. If there is no quadruple  $q$  in  $Q$  beginning with  $a(v, -)$ , then the completed action of the next step, given by  $\exp(-\frac{1}{2}i\pi H_2^Q)$  acting on  $\Psi_Q^{int}(t)$ , is given by the  $1 - P_Q$  term of Eq. (24). That is, if  $t'$  is such that  $t' > t$ ,  $n(t') = n(t) + 1$ , and  $\Psi_Q^{int}(t')$  is stationary, then

$$\Psi_Q^{int}(t') = (1 - P_Q)\Psi_Q^{int}(t)$$

Thus no computation step is carried out. From here on  $\Psi_Q^{int}(t)$  evolves by shifting  $H_R$ , copying, and doing nothing, in sequence, until  $t > 3Nd + w + r$ . At this time  $\Psi_Q^{int}(t)$  becomes permanently stationary. Thus in this case, since no calculating is occurring, the last part of the record consists of repeated copying of the final machine internal state, scanned symbol, and  $H_C$  position.

For a standard Turing machine  $Q$  with the initial state  $\Psi_Q^{\text{int}}(0)$  in the standard form, this halting condition will arise if the final machine state  $a_f$  appears before  $3N$  model steps have occurred. In this case the Turing machine calculating is completed in less than  $N$  steps. Such a situation can also arise if  $\Psi_Q^{\text{int}}(0)$  is not in the standard form, e.g., if one starts out with the machine in an internal state different from  $a_i$ .

### 6. DISCUSSION

There are several aspects of the models constructed here which should be noted. First, one notes that, contrary to what might have been expected, it is possible to construct a quantum mechanical model of a decision procedure. The construction is valid in the sense that record, act, and shift steps are all described by interaction Hamiltonians. In particular the necessary correlation required by “read the record, if  $\alpha$  is read, carry out operation  $O_\alpha$  on the system” is already built into the Hamiltonian. The whole process can be described by a pure state evolving under the action of such a Hamiltonian. Of course the possibility of such a construction is conditioned on the approximations used in the models developed here.

In order to compare the models constructed here with those of Landauer<sup>(13)</sup> and with real computers so far built, it is helpful to evaluate the contributions of various terms to the total energy. By use of Eqs. (28)–(30) and (40)–(43) one can show that the total energy ( $\Psi(t)$ ,  $H\Psi(t)$ ) (the  $Q$  and  $N$  indices are suppressed) consists of the sum of two terms each given by

$$(\Psi(t), H_0\Psi(t)) = 3N \int_{-\infty}^{\infty} \varphi^*(x) \frac{1}{i} \frac{\partial}{\partial x} (\varphi(x)) dx - (\varphi\Psi^{\text{int}}, VH(n(t))\varphi\Psi^{\text{int}})_{n(t)} \tag{49}$$

and

$$(\Psi(t), H'\Psi(t)) = (\varphi\Psi^{\text{int}}, VH(n(t))\varphi\Psi^{\text{int}})_{n(t)} \tag{50}$$

Here

$$\begin{aligned} &(\varphi\Psi^{\text{int}}, VH(n(t))\varphi\Psi^{\text{int}})_{n(t)} \\ &= \int_{-\infty}^{\infty} \varphi^*(x_{n(t)} + n(t)d - t)V(x_{n(t)})\varphi(x_{n(t)} + n(t)d - t) dx_{n(t)} \\ &\quad \times [\Psi^{\text{int}}(n(t) - 1)H(n(t))\Psi^{\text{int}}(n(t) - 1)] \end{aligned} \tag{51}$$

and

$$\Psi^{\text{int}}(n(t) - 1) = e^{-i\pi H(n(t)-1)/2} \dots e^{-i\pi H_1/2}\Psi^{\text{int}}(0) \tag{52}$$

It is clear from the above that the total energy equals that carried by the control systems,  $3N$  times the kinetic energy of a single control system. Also, it turns out that, for standard machine initial states of the form given by Eq.

(40), the interaction energy  $(\Psi(t), H'\Psi(t)) = 0$  for all times  $t$  for which either no control system is interacting with  $M$   $\{n(t)d + w + r \leq t < [n(t) + 1]d - w - r$  if  $n(t) < 3N$ , or  $3Nd + w + r < t$  if  $n(t) = 3N\}$  or if  $t$  is such that  $n(t) \bmod 3 = 1$  or  $2$ . This latter condition arises from the fact that if the structure of the interaction Hamiltonians, Eqs. (14) and (15), for the record and compute types of steps is such that, if  $\Psi^{\text{int}}(0)$  has the form given by Eq. (40), then  $(\Psi^{\text{int}}(n(t) - 1), H(n(t))\Psi^{\text{int}}(n(t) - 1)) = 0$  if  $H(n(t)) = H_1$  or  $H_2$ . Only for the third type of step, which is the shift of the recording head and which occurs only when  $n(t) \bmod 3 = 0$  and  $(\varphi, V\varphi)_{n(t)} \neq 0$ , does one have, by Eqs. (16), (20), (30), and (40),

$$(\Psi^{\text{int}}(n(t) - 1), H(n(t))\Psi(n(t) - 1)) = (\psi_l^H, B\psi_l^H)$$

where  $l =$  largest integer contained in  $[n(t) + 2]/3$ .

It follows from these results that at all times after the completion of a model step and before the beginning of the next, or after  $3N$  steps, the energy of the control systems is the same as it is at the beginning, and the interaction energy is zero. There is no net transfer of energy to the Turing machine part  $(M + H_c + T + H_r + R)$  as the calculation progresses.

In this respect the models discussed here are different from those discussed by Landauer<sup>(13)</sup> in that in his models the computation process dissipates energy at each step. Furthermore, the energy dissipation can be arbitrarily small if the computation process is sufficiently slow. No such limitation exists for the models constructed here. They proceed at a finite speed and dissipate zero energy.

The models constructed here are also quite different from those discussed by Landauer<sup>(13)</sup> and from real computers so far constructed in that they are models of what might be called a "coherent" computer or computation process. That is, the whole computation process is described by a pure state evolving under the action of a given Hamiltonian. Thus all the component parts of the Turing machine are described by states which have a definite phase relation to one another as the calculation progresses [Eqs. (23) and (26)].

The existence of such models at least suggests that the possibility of actually constructing such coherent machines should be examined. Such machines would have the advantage that there is no energy dissipation and resultant heat buildup, which are problems in the large computers. On the other hand, the model Hamiltonians constructed here are very complex. As a result it is difficult to conceive how one would actually build such a machine.

The models constructed here do in fact require some energy dissipation. However, this occurs only at the times the operator examines the machine to see if the computation is finished and if so, to restore the Turing machine to

the initial state. However, when and where and how much energy is so dissipated is under external control. It is not part of the computation process itself. This will be discussed more in another paper.

In this connection it should be noted that for the models constructed here both the system carrying the information and the machine that reads and acts on the system are considered as interacting quantum systems. The entire complexity of the computation process resides in the complexity of the interaction. The system evolves in isolation from the external world. Reading the overall state of the model system, which includes reading the computation tape, is an interaction with the external world. It does not perturb the wave function provided it is done in the intervals  $\Delta$  centered on the times  $t_1, \dots, t_{3N}$ . Thus there is no "reduction of the wave packet" for reading done in these time intervals.

In conclusion it must be stressed again that the existence of such models was shown here by the use of the Coleman model approximation.<sup>(6,18)</sup> This model has the consequence that the model Hamiltonian evolution is clean, with no interference between component states representing different computation steps. The reason is that the control system wave packets do not spread as they move past  $M$ . As a result there is no interference between the different model step states as the system evolves.

Use of the correct  $\nabla^2/2m$  would give wave packet spreading and a resultant interference between different model steps because the machine  $M$  would interact with several control systems at once. However, by suitable choice of external parameters, the control system wave packet spreading can be kept quite small. It may be, though, that this will result in a slowing down of the model computation process by spacing the successive control systems farther and farther apart to keep the interference effects quite small.

It has been shown here that, if the Coleman model is used, for each  $N$  and Turing machine  $Q$ , one can construct a quantum mechanical Hamiltonian model for  $\leq N$  computation steps which creates and saves a history tape. It leaves open the question of whether it is possible to construct a Hamiltonian model which erases its own history tape and whether models can be constructed for the limit  $N = \infty$ . It is hoped to investigate both these problems in a future paper.

## APPENDIX

The problem is to obtain the solution to the Schrödinger equation as given by Eqs. (41) and (42) if  $H_Q$  is given by Eqs. (28)–(31), or

$$H_Q = H_0 + H' \tag{A1}$$

where (the  $Q$  indices are suppressed) by the Coleman model assumption

$$H_0 = \sum_{j=1}^{3N} \frac{1}{i} \frac{\partial}{\partial x_j} \tag{A2}$$

and

$$H' = \sum_{j=1}^{3N} V(x_j)H'(j) \tag{A3}$$

with

$$H'(j) = \begin{cases} H_1 & 1 = j \bmod 3 \\ H_2 & \text{if } 2 = j \bmod 3 \\ H_3 & 0 = j \bmod 3 \end{cases} \tag{A4}$$

and  $H_1$ ,  $H_2$ , and  $H_3$  are given by Eqs. (14)–(16). Also,  $V(x_j)$  is such that  $\int_{-\infty}^{\infty} V(x) dx = \pi/2$ , and  $V(x) = 0$  if  $|x| > r$ . The initial state  $\Psi_Q(0)$  is given by Eq. (39) as

$$\Psi_Q(0) = \Psi^C(0, x, \dots, x_{3N})\Psi_Q^{\text{int}}(0) \tag{A5}$$

with

$$\Psi^C(0, x, \dots, x_{3N}) = \bigotimes_{j=1}^{3N} \varphi(x_j + jd) \tag{A6}$$

where  $\varphi(z) = 0$  if  $|z| > w$ , and the packet separation distance  $d$  satisfies  $d > 2r + 2w$ .

One has from the Schrödinger equation<sup>(20)</sup>  $i d\Psi(t)/dt = (H_0 + H')\Psi(t)$

$$e^{-iHt} = e^{-iH_0t} - i \int_0^t e^{-iH_0(t-\tau)} H' e^{-iH\tau} d\tau \tag{A7}$$

Successive iterations give the expansion<sup>(20)</sup>

$$e^{-iHt} = e^{-iH_0t} + \sum_{n=1}^{\infty} (-i)^n \int_0^t d\tau_1 e^{-iH_0(t-\tau_1)} H' \dots \\ \times \int_0^{\tau_{n-1}} e^{-iH_0(\tau_n - \tau_{n-1})} H' e^{-iH_0\tau_n} d\tau_n$$

This expansion converges uniformly if  $H'$  is bounded,<sup>(20)</sup> which is clearly the case here [ $N$  is finite and  $H(j)$ , which is independent of  $x_j$ , consists of finite sums of products of spin operators and shift operators].

Use of the fact that

$$e^{-iH_0a} H' = H'(a) e^{-iH_0a} \tag{A8}$$

where

$$H'(a) = \sum_{j=1}^{3N} V(x_j - a)H'(j) \tag{A9}$$



gives

$$e^{-iHt} = V(t) e^{-iH_0 t} \tag{A10}$$

where

$$V(t) = \sum_{n=0}^{\infty} (-i)^n \int_0^t d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n H'(t - \tau_1) H'(t - \tau_2) \cdots H'(t - \tau_n) \tag{A11}$$

and the  $n = 0$  term is equal to 1.

This gives

$$\begin{aligned} \Psi_Q(t, x_1, \dots, x_{3N}) &= V(t) e^{-iH_0 t} \Psi^C(0, x_1, \dots, x_{3N}) \Psi_Q^{\text{int}}(0) \\ &= \bigotimes_{j=1}^{3N} \varphi(x_j + jd - t) V(t) \Psi_Q^{\text{int}}(0) \end{aligned} \tag{A12}$$

Consider, using Eqs. (A9) and (A11), a general term in (A12). It will have the form

$$\begin{aligned} &\bigotimes_{j=1}^{3N} \varphi(x_j + jd - t) \int_0^t d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n \\ &\times [V(x_{j_1} - t + \tau_1) H'(j_1) \cdots V(x_{j_n} - t + \tau_n) H'(j_n)] \Psi_Q^{\text{int}}(0) \end{aligned}$$

From the restrictions on  $\varphi$ ,  $d$ , and  $V$  given, along with  $\tau_{j+1} \leq \tau_j, j = 1, 2, \dots, n$ , one can show that this term is zero for all  $x_{j_1}, \dots, x_{j_n}$  unless  $j_1 \geq j_2 \geq \dots \geq j_n$ . To see this, consider any pair of indices  $j_k$  and  $j_l$  with  $k < l$ . Associated with these indices is the factor

$$\varphi(x_{j_k} + j_k d - t) V(x_{j_k} - t + \tau_k) \varphi(x_{j_l} + j_l d - t) V(x_{j_l} - t + \tau_l)$$

This factor is nonzero if

$$\begin{aligned} -w &\leq x_{j_k} + j_k d - t \leq w, & -r &\leq x_{j_k} - t + \tau_k \leq r \\ -w &\leq x_{j_l} + j_l d - t \leq w, & -r &\leq x_{j_l} - t + \tau_l \leq r \end{aligned}$$

From the first pair of double inequalities one can eliminate  $x_{j_k} - t$  to obtain  $-r + \tau_k \leq w + j_k d$ . From the second pair one can eliminate  $x_{j_l} - t$  to obtain  $-w + j_l d \leq r + \tau_l$ . These two can be added and rearranged to give

$$j_l d - j_k d \leq \tau_l - \tau_k + 2w + 2r \leq 2w + 2r$$

since  $\tau \geq \tau_l$ . But this implies  $j_k - j_l \leq 0$  or  $j_k \leq j_l$  as  $d > 2w + 2r$ .

As a result, the only nonzero contributions to  $\Psi_Q(r, x_1, \dots, x_{3N})$  come

from those terms for which the control system labels do not decrease as one moves to the left in the general term. Thus one has

$$\Psi_Q(t, x_1, \dots, x_{3N}) = \bigotimes_{j=1}^{3N} \varphi(x_j + jd - t) \sum_{n=0}^{\infty} (-i)^n \int_0^t d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n \times \sum_{j_1=1}^{3N} Y_{j_1}(\tau_1 x_{j_1}) \sum_{j_2=1}^{j_1} Y_{j_2}(\tau_2 x_{j_2}) \cdots \sum_{j_n=1}^{j_{n-1}} Y_{j_n}(\tau_n x_{j_n}) \Psi_Q^{\text{int}}(0) \tag{A13}$$

where

$$Y_{j_i}(\tau_i x_{j_i}) = V(x_{j_i} - t + \tau_i) H'(j_i) \tag{A14}$$

Note that the different  $Y$  factors do not commute in general.

Consider next the factors in (A13) containing  $j_1, \varphi(x_{j_1} + j_1 d - t) V(x_{j_1} - t + \tau_1)$ . Proceeding as before and eliminating  $x_{j_1} - t$  from the double inequalities, one finds that this term is nonzero for some  $x_{j_1}$  iff  $\tau_1 - w - r \leq j_1 d \leq \tau_1 + w + r$ . Now  $0 \leq \tau_1 \leq t$ . Thus this factor is nonzero if  $j_1 d \leq t + w + r$ . Define  $n(t)$  by  $n(t) =$  smaller of  $3N$  or the maximum value of  $j$  such that  $jd \leq t + w + r$ . One can replace the upper limit of the  $j_1$  sum by  $n(t)$  to get

$$V(t) \Psi_Q^{\text{int}}(0) = \sum_{n=0}^{\infty} (-i)^n \int_0^t d\tau_1 \cdots \int_0^{\tau_{n-1}} d\tau_n \sum_{j_1=1}^{n(t)} Y_{j_1}(\tau_1 x_{j_1}) \cdots \times \sum_{j_n=1}^{j_{n-1}} Y_{j_n}(\tau_n x_{j_n}) \Psi^{\text{int}}(0) \tag{A15}$$

Consider a general term  $Y_{j_1}(\tau_1 x_{j_1}) \cdots Y_{j_n}(\tau_n x_{j_n})$  of Eq. (A15). Let  $l_1$  be the number of  $Y$  factors whose  $j$  indices are  $1; \dots; l_m$  be the number of  $Y$  factors whose  $j$  indices are  $m; \dots; \text{and } l_{n(t)}$  be the number of  $Y$  factors whose  $j$  indices are  $n(t)$ . [From the structure of the  $j$  sums there are at most  $n(t)$  distinct  $j$  values.] For a particular term  $l_m = 0$  if  $Y_m$  does not appear in it. Since the  $j_1, \dots, j_n$  sequence is nonincreasing from left to right, all  $l_m$  of the  $Y_m$  factors stand to the right of the number  $l_{m+1}$  of the  $Y_{m+1}$  factors. One can then replace the  $n$  sum and all the  $j$  sums by sums over  $l_1, \dots, l_{n(t)}$ . After making corresponding changes in the indices of the  $\tau$  variables, one obtains

$$V(t) \Psi_Q^{\text{int}}(0) = \sum_{l_{n(t)}=0}^{\infty} (-i)^{l_{n(t)}} \int_0^t d\tau_1 \cdots \int_0^{\tau_{l_{n(t)}-1}} d\tau_{l_{n(t)}} \times [Y_{n(t)}(\tau_1 x_{n(t)}) \cdots Y_{n(t)}(\tau_{l_{n(t)}} x_{n(t)})] \times \sum_{l_{n(t)-1}=0}^{\infty} (-i)^{l_{n(t)-1}} \int_0^{\tau_{l_{n(t)}}} d\tau_{l_{n(t)+1}} \cdots \int_0^{\tau_{\alpha}-1} d\tau_{\alpha} \times [Y_{n(t)-1}(\tau_{l_{n(t)+1}} x_{n(t)-1}) \cdots Y_{n(t)-1}(\tau_{\alpha} x_{n(t)-1})] \times \cdots \sum_{l_1=0}^{\infty} (-i)^{l_1} \int_0^{\tau_{\beta}} d\tau_{\beta+1} \cdots \int_0^{\tau_{\beta+l_1}-1} d\tau_{\beta+l_1} \times [Y_1(\tau_{\beta+1} x_1) \cdots Y_1(\tau_{\beta+l_1} x_1)] \Psi_Q^{\text{int}}(0) \tag{A16}$$

where  $\alpha = l_{n(t)} + l_{n(t)-1}$  and  $\beta = l_{n(t)} + l_{n(t)-1} + \dots + l_2$  are used as temporary notation.

In writing Eq. (A16) the following convention has been used for each  $j = 0, 1, \dots, n(t)$ . For the  $l_j = 0$  term in the  $l_j$  sum the entire square bracket containing the  $Y_j$  factors and the integrals is to be replaced by 1. After this convention is applied, any  $\tau_0$  appearing as an upper limit is to be replaced by  $t$ .

Next, consider the  $l_1$  sum. One can, by following the methods developed by Dyson,<sup>(21)</sup> replace the upper limits of all the integrals by  $\tau_\beta$  provided a normalizing factor of  $(l_1!)^{-1}$  is included. No time ordering operator is needed, since all the  $Y_1$  factors commute. One has as a result

$$\sum_{l_1=0}^{\infty} (-i)^{l_1} \int_0^{\tau_\beta} d\tau_{\beta+1} \dots d\tau_{\beta+l_1} [Y_1(\tau_{\beta+1} x_1) \dots Y_1(\tau_{\beta+l_1} x_1)] = \exp\left[-iH_1 \int_{x_1-t}^{x_1-t+\tau_\beta} V(z) dz\right] \tag{A17}$$

where  $Y_1(\tau x_1) = V(x_1 - t + \tau)H_1$  has been used along with a variable change  $z = x_1 - t + \tau$ .

The  $l_1$  sum in Eq. (A16) is multiplied on the left by  $Y_2(\tau_\beta x_2)$ . Bringing in the two relevant wave packets, one sees that Eq. (A16) contains the factor

$$\varphi(x_1 + d - t)\varphi(x_2 + 2d - t)V(x_2 - t + \tau_\beta) \exp\left[-iH_1 \int_{x_1-t}^{x_1-t+\tau_\beta} V(z) dz\right]$$

common to all terms in the  $l_{n(t)}, \dots, l_2$  sums. This factor is different from zero iff  $-w \leq x_1 + d - t \leq w$ ,  $-w \leq x_2 + 2d - t \leq w$ , and  $-r \leq x_2 - t + \tau_\beta \leq r$ . Elimination of  $x_2 - t$  from the last two double inequalities gives  $-r - w + 2d \leq \tau_\beta \leq r + w + 2d$ . Use of this with the first double inequality gives  $-x_1 - t + \tau_\beta \geq d - 2w - 2r > r$  as  $d > 2w + 2r$ . Similarly  $x_1 - \tau \leq w - d < r$ .

As a result, the upper and lower limits of the integral in the exponent can be replaced by  $r$  and  $-r$ . This gives

$$\exp\left[-iH_1 \int_{x_1-t}^{x_1-t+\tau_\beta} V(z) dz\right] = \exp(-\frac{1}{2}i\pi H_1) \tag{A18}$$

which then replaces the  $l_1$  sum in Eq. (A16).

Since  $\exp(-\frac{1}{2}i\pi H_1)$  is independent of  $\tau_\beta$ , one can repeat the above argument on the  $l_2$  sum and obtain

$$\sum_{l_2=0}^{\infty} (-i)^{l_2} \int_0^{\tau_\beta} d\tau_{\gamma+1} \dots \int_0^{\tau_\beta+l_2-1} d\tau_{\gamma+l_2} \times [Y_2(\tau_{\gamma+1}x_2) \dots Y_2(\tau_{\gamma+l_2}x_2)]e^{-i\pi H_1/2} = e^{-i\pi H_2/2} e^{-i\pi H_1/2} \tag{A19}$$

where  $\gamma = l_{n(t)} + \dots + l_3$ . Proceeding in this fashion, one can proceed leftward through Eq. (A16) replacing the  $l_j$  sum factor by  $\exp[-\frac{1}{2}i\pi H'(j)]$ , where  $H'(j)$  is given in Eq. (A4), until one comes to the  $l_{n(t)}$  sum. For this case the above argument gives the factor

$$\exp\left[-iH'(n(t)) \int_{x_{n(t)}-t}^{x_{n(t)}} V(z) dz\right]$$

which is multiplied by  $\varphi(x_{n(t)} + n(t)d - t)$  in the full expression. Again one can replace the lower limit by  $-r$  (or  $-\infty$ ) to get

$$\exp[-iH'(n(t))F(x_{n(t)})]$$

where  $F(x_{n(t)})$  is given by  $\int_{-\infty}^{x_{n(t)}} V(r) dr$  as a replacement for the  $l_{n(t)}$  sum factors.

Putting these results together, one finally obtains

$$\begin{aligned} \Psi_Q(t, x_1, \dots, x_{3N}) &= \bigotimes_{j=1}^{3N} \varphi(x_j + jd - t) \exp[-iH'(n(t))F(x_{n(t)})] \\ &\times \exp[-\frac{1}{2}i\pi H'(n(t) - 1)] \dots \exp[-\frac{1}{2}i\pi H_1] \Psi_Q^{\text{int}}(0) \end{aligned} \tag{A20}$$

which is the desired equation (41) of the text.

From the requirement that

$$\varphi(x_{n(t)} + n(t)d - t) \exp[-iH'(n(t))F(x_{n(t)})]$$

be different from zero, one obtains

$$w - n(t)d + t \geq x_{n(t)} \geq -w - n(t)d + t$$

If  $t$  is such that  $t \geq r + w + n(t)d$ , then  $F(x_{n(t)}) = \pi/2$  for all  $x_{n(t)}$  for which  $\varphi(x_{n(t)} + n(t)d - t) \neq 0$ . Since this holds in particular for all  $t \geq r + w + 3Nd$ , one has Eq. (42).

It is to be emphasized that the derivation of Eq. (A20) depends essentially on the restrictions that the wave packets and potential have compact support and  $d > 2w + 2r$ . If any of these restrictions is relaxed,  $\Psi_Q(t, x_1, \dots, x_{3N})$  can no longer be written as a simple product of exponentials acting on  $\Psi_Q^{\text{int}}(0)$ .

### ACKNOWLEDGMENTS

The author wishes to thank Hans Ekstein and the CNRS, Centre de Physique Theorique, Luminy, for their hospitality and support during the visit in which this work was completed.

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