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Quantum hopping models for kinetic processes

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We propose that a quantum operator, apart from representing quantum dynamics, may also represent a dynamical (steady-state) situation of a classical system. We consider a Hamiltonian that describes hopping of single (spinless, noninteracting) bosons to nearest-neighbor sites in a hypercubic lattice and find exactly the mass distribution (in arbitrary dimension) for the ground state and the first excited state. The density shows a peak at a mass equal to the density. A variant of this Hamiltonian is shown to have an exponential mass distribution (in the ground state) that is identical with an analogous classical model.

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Investigation of the steady state for kinetic models had always been a matter of interest. Such models have been shown to represent in some way the processes of aggregation and desorption [1–5], thin film deposition [6], catalytic reactions [7], evolution in a tank reactor [8], kinetics of polymerization [9], etc. However, all these models refer to a classical system and basically consists of choosing an updating rule that converts the configuration of a system from one to another. One starts with a trial configuration and operates the rule repeatedly until the system reaches a “steady state” in the sense that an average of some physical property over several successive configurations becomes constant. In this Brief Report we propose that a *quantum* operator, apart from representing quantum dynamics, may also represent a dynamical (steady-state) situation of a classical system. For a quantum system, let $|\psi\rangle$ be some state that is a superposition of many configurations. The measured value of a physical quantity in this state will represent a weighted average over the constituent configurations. If we operate repeatedly on $|\psi\rangle$, some operator \mathcal{H} that incorporates some physical process of interest, then this average will go on changing until the eigenstate is reached. The eigenstate will be invariant under the physical process described by the operator. The study of the eigenstates of quantum Hamiltonians will therefore enrich our knowledge about classical kinetic situations.

To illustrate this point further, let us consider the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{r}, \mathbf{n}} c_{\mathbf{r}}^{\dagger} c_{\mathbf{r}+\mathbf{n}} \quad (1)$$

that describes hopping of single (spinless, noninteracting) bosons to nearest-neighbor sites in some d -dimensional hy-

percubic lattice $\{\mathbf{r}\}$. (Here, $c_{\mathbf{r}}, c_{\mathbf{r}}^{\dagger}$ are the destruction and creation operators for bosons and \mathbf{n} runs over the nearest-neighbor positions.) An eigenstate of this Hamiltonian will, in general, be a superposition of many configurations and will in some sense be invariant under boson hopping.

For the classical models, the quantity studied has often been the mass distribution function. Usually the power law or exponential decay is observed [1–5,8,9], but recently a peak at a high mass (after the tail of algebraic decay) has also been found [5]. Below, we shall determine exactly (in arbitrary dimension) the ground-state mass distribution for the Hamiltonian \mathcal{H} mentioned above. The number of bosons at a site \mathbf{r} is called as the mass at \mathbf{r} and the mass distribution function $P(m)$, ($m=0,1,2,\dots$) is defined as the probability

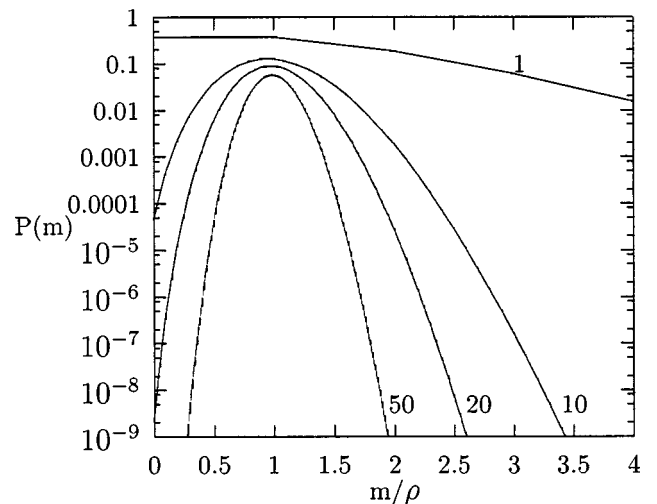


FIG. 1. Mass distribution [Eq. (6)] for the ground state of the Hamiltonian \mathcal{H} . The numbers in the figure indicate the density. All curves are for $N=1000$, but the curves are highly insensitive to the value of N .

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of getting exactly m particles at any site in the lattice $\{\mathbf{r}\}$. It is found that the function $P(m)$ has the interesting property that for density (say, ρ) lower than 1, $P(m)$ decreases monotonically with m , while for $\rho > 1$, $P(m)$ shows a peak (Fig. 1). In this sense, there is some sort of a transition at $\rho = 1$. Although such peaks are uncommon for the classical models studied so far, one must note that it has been observed experimentally long ago [10] in Au clusters on NaCl and Ag clusters on C.

One crucial question is the following: to what classical situation does the ground state of \mathcal{H} correspond? One immediately suggestive updating rule (for classical systems) is the following.

\mathcal{C} : Choose a site i randomly, remove one particle from this site, among the nearest neighbors of i choose one neighbor randomly and add one particle to this neighbor.

It will be seen below that this rule gives a mass distribution that is simply exponential and hence does not agree with that for the ground state of \mathcal{H} . This disagreement is presumably due to the presence of the mass amplitudes in the definition of boson operators:

$$c|m\rangle = \sqrt{m}|m-1\rangle, \quad c^\dagger|m\rangle = \sqrt{m+1}|m+1\rangle.$$

We shall therefore also analyze a somewhat different Hamiltonian for hopping bosons, viz.,

$$\mathcal{H}' = - \sum_{\mathbf{r}, \mathbf{n}} [a_{\mathbf{r}}^\dagger a_{\mathbf{r}+\mathbf{n}} + \delta_{m(\mathbf{r}),0}]. \quad (2)$$

Here, $a_{\mathbf{r}}, a_{\mathbf{r}}^\dagger$ are the destruction and creation operators for bosons with amplitude 1,

$$a|m\rangle = |m-1\rangle, \quad a^\dagger|m\rangle = |m+1\rangle, \quad a|0\rangle = 0,$$

$m(\mathbf{r}) = c_{\mathbf{r}}^\dagger c_{\mathbf{r}}$ and other notations are the same as above. \mathcal{H}' is also a quantum operator, since a, a^\dagger do not commute:

$$[a_{\mathbf{r}}, a_{\mathbf{r}}^\dagger] = \delta_{m(\mathbf{r}),0}.$$

For \mathcal{H}' , the ground state mass distribution is found to be exponentially decaying and precisely identical to that for \mathcal{C} . Thus, although the classical analogue of \mathcal{H} could not be determined, the same for \mathcal{H}' is found to be nothing but \mathcal{C} .

We shall now determine the mass distribution for \mathcal{H} . We first note that the total number of bosons M and hence the density $\rho = M/N$, N being the total number of sites, is conserved. It is easy to observe that by Fourier transformation to the boson operators

$$c_{\mathbf{q}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} c_{\mathbf{r}} \exp(i\mathbf{q} \cdot \mathbf{r})$$

under periodic boundary condition, one can immediately diagonalize this Hamiltonian to

$$\mathcal{H} = \sum_{\mathbf{q}, \mathbf{n}} c_{\mathbf{q}}^\dagger c_{\mathbf{q}} \cos(\mathbf{q} \cdot \mathbf{n}).$$

Here $\{\mathbf{q}\}$ is the reciprocal lattice of $\{\mathbf{r}\}$ with the convention that $0 < \mathbf{q} \cdot \mathbf{n} \leq 2\pi$. The ground state is one for which all the M particles are at $q = \pi$ for one-dimensional lattice, at \mathbf{q}

$= (\pi, \pi)$ for square lattice, and at $\mathbf{q} = (\pi, \pi, \pi)$ for cubic lattice. We now note that due to translational symmetry, the quantity $P(m)$ is the same as the probability $P_{\mathbf{r}}(m)$ of getting m particles at some specific site \mathbf{r} . To obtain $P_{\mathbf{r}}(m)$ in some state $|\psi\rangle$ we resolve the state into the component boson distributions in the original space $\{\mathbf{r}\}$:

$$|\psi\rangle = \sum_k A(k)|k\rangle$$

and then observe that

$$P_{\mathbf{r}}(m) = \sum_k |A(k)|^2 \delta_{m(\mathbf{r},k),m}, \quad (3)$$

where $m(\mathbf{r},k)$ is the mass at the site \mathbf{r} in the distribution $|k\rangle$. We shall now calculate the quantity

$$b_m = \langle \psi | (c_{\mathbf{r}}^\dagger)^m (c_{\mathbf{r}})^m | \psi \rangle. \quad (4)$$

As we operate $(c_{\mathbf{r}})^m$ on $|k\rangle$, two situations may arise; the states for which $m(\mathbf{r},k) < m$ will be annihilated and the states with $m(\mathbf{r},k) \geq m$ will be converted to one with amplitude

$$\{m(\mathbf{r},k)(m(\mathbf{r},k)-1)(m(\mathbf{r},k)-2) \cdots (m(\mathbf{r},k)-m+1)\}^{1/2}$$

having $(m(\mathbf{r},k)-m)$ particles at the site \mathbf{r} . This gives

$$b_m = \sum_{j=m}^M \sum_k |A(k)|^2 \frac{j!}{(j-m)!} \delta_{m(\mathbf{r},k),j}$$

and substituting Eq. (3) here we have

$$b_m = \sum_{j=m}^M \frac{j!}{(j-m)!} P(j).$$

This equation is quite general and can be easily inverted by calculating the generating function. Thus, we multiply both sides by $(x-1)^m/m!$, sum over m from 0 to M , and compare the coefficient of x^j from both sides to obtain

$$P(j) = \sum_{m=j}^M \frac{(-1)^{m-j}}{m!} \binom{m}{j} b_m, \quad (5)$$

where $\binom{m}{j}$ is the binomial coefficient. If one can find b_m by applying Eq. (4) on a given state $|\psi\rangle$, then Eq. (5) gives immediately the mass distribution function $P(j)$. Let us first apply this procedure to the state where all the particles are at some $\mathbf{q} = \mathbf{q}_0$. The ground state of \mathcal{H} is one such state. Writing $(c_{\mathbf{r}}^\dagger)^m (c_{\mathbf{r}})^m$ as

$$\frac{1}{N^m} \sum_{\mathbf{q}_1, \mathbf{q}'_1=0}^{2\pi} c_{\mathbf{q}'_1}^\dagger c_{\mathbf{q}_1}^\dagger \cdots c_{\mathbf{q}'_m}^\dagger c_{\mathbf{q}_1} c_{\mathbf{q}_2} \cdots c_{\mathbf{q}_m} \\ \times \exp[i\mathbf{r} \cdot (\mathbf{q}'_1 + \mathbf{q}'_2 + \cdots + \mathbf{q}'_m - \mathbf{q}_1 - \mathbf{q}_2 \cdots - \mathbf{q}_m)]$$

we note that $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_m$ all must be equal to \mathbf{q}_0 , since only this state is occupied. Moreover, each of $\mathbf{q}'_1, \mathbf{q}'_2, \dots, \mathbf{q}'_m$ must also be \mathbf{q}_0 , since otherwise we do not get back the original state $|\psi\rangle$. This gives

$$b_m = \frac{1}{N^m} \frac{M!}{(M-m)!}$$

and substituting this expression in Eq. (5) one gets the final expression for the ground-state mass distribution of \mathcal{H} :

$$P(m) = \frac{(N-1)^{M-m}}{N^M} \binom{M}{m}. \quad (6)$$

One immediately obtains the equality

$$\frac{P(m)}{P(m-1)} = \frac{M+1-m}{mN-m},$$

which implies that $P(m)$ increases with m for $m < (M+1)/N \sim \rho$, reaches a peak at $m = \rho$, and then decreases, giving an asymmetric Gaussian-type curve (Fig. 1). Also, there will be no peak for $(M+1) < N$, or $\rho < 1$.

In the first excited state, one particle (in $\{\mathbf{q}\}$ space) will be removed from the ground state and put to some other state, \mathbf{q}' , say. To calculate b_m now, we note that \mathbf{q}' may be equal to any or none of $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_m$ as well as $\mathbf{q}'_1, \mathbf{q}'_2, \dots, \mathbf{q}'_m$. This gives

$$b_m = \frac{1}{N^m} \frac{M!}{(M-m)!} \left(1 - \frac{m}{M} + \frac{m^2}{M} \right).$$

Straightforward calculation then gives

$$P(m) = \frac{(N-1)^{M-m}}{N^M} \binom{M}{m} \frac{1}{M(M-1)} \times \left[\frac{1}{(N-1)^2} (M-m)(M-m-1)(N^2 - 2N + M) + \frac{2}{N-1} m(M-m)(N-M) + Mm(m-1) \right]$$

for $0 \leq m < M-2$ and $P(M-1) = [M(M-2)(N-1) - 2M + 2N]/N^M$, $P(M) = M/N^M$.

Another state that can be tackled in closed form is one for which one particle is in each of M states (in $\{\mathbf{q}\}$ space) (assuming that $\rho < 1$). Noting that the m particles to be destroyed by the c operators can be chosen in $\binom{M}{m}$ ways, and that the m particles chosen may be distributed in $m!$ ways among $\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_m$ as well as $\mathbf{q}'_1, \mathbf{q}'_2, \dots, \mathbf{q}'_m$, we get

$$b_m = \frac{(m!)^2}{N^m} \binom{M}{m}$$

and

$$P(m) = \sum_{j=m}^M \frac{(-1)^{j-m}}{N^j} \binom{M}{j} \binom{j}{m} j!$$

This sum cannot be evaluated easily. Instead, one can derive from this equation the equality

$$P(m) = P(m+1) + \frac{N}{M+1} P_{M+1}(m+1),$$

where $P_{M+1}(m+1)$ is the function $P(m+1)$ when the total mass is $(M+1)$. However, since for large M we may assume $P_{M+1}(m+1) \sim P(m+1)$, we obtain herefrom an *exponential* distribution:

$$P(m) = \frac{1}{\rho+1} \left(\frac{\rho}{\rho+1} \right)^m. \quad (7)$$

A few comments are in order. (i) The distribution of particles in the $\{\mathbf{q}\}$ space indeed determines the mass distribution in $\{\mathbf{r}\}$ space, but not so sensitively. Thus, when masses m_1, m_2, \dots are at states $\mathbf{q}_1, \mathbf{q}_2, \dots$, respectively, the numbers m_1, m_2, \dots alone determine the distribution $P(m)$ in the space $\{\mathbf{r}\}$, and the specific values of $\mathbf{q}_1, \mathbf{q}_2, \dots$ do not matter. For example, all the states that have all particles in *one* state will not have the same energy, but will have the same $P(m)$ as the ground state. (ii) At least for this Hamiltonian, it is difficult to find whether the mass distribution reflects a phase transition or not. Thus, it is easy to see that the Hamiltonian \mathcal{H} undergoes a Bose condensation (although only in three-dimensions), but it is difficult to calculate the mass distribution across the transition temperature, or for that matter, at any nonzero temperature. (iii) One can easily calculate the quantity

$$(c_{\mathbf{r}}^\dagger c_{\mathbf{r}})^2 = \frac{1}{N^2} \sum_{\mathbf{q}_i=0}^{2\pi} c_{\mathbf{q}_1}^\dagger c_{\mathbf{q}_2} c_{\mathbf{q}_3}^\dagger c_{\mathbf{q}_4} \exp[i\mathbf{r} \cdot (\mathbf{q}_1 - \mathbf{q}_2 + \mathbf{q}_3 - \mathbf{q}_4)]$$

in any of the states considered above, and calculate therefrom the ‘‘roughness parameter’’

$$\langle (c_{\mathbf{r}}^\dagger c_{\mathbf{r}})^2 \rangle - \langle c_{\mathbf{r}}^\dagger c_{\mathbf{r}} \rangle^2.$$

This quantity remains finite always. For example, it is simply ρ and $\rho^2 + \rho$, respectively for the ground state and for the state that has one particle in each of M states.

We now analyze the Hamiltonian \mathcal{H}' for hopping bosons defined by Eq. (2). Let us define $|0\rangle$ as the state that is a superposition of all possible distributions of M bosons among N sites. This state can be shown to be the ground state of \mathcal{H}' by proving that (i) this state is an eigenstate of $-\mathcal{H}'$ with eigenvalue $2dN$ and (ii) the numerically largest eigenvalue of $-\mathcal{H}'$ is $2dN$. To prove (i), we observe that if $|k\rangle$ is a configuration with no vacant site, then $a_{\mathbf{r}}^\dagger a_{\mathbf{r}+\mathbf{n}}|k\rangle$ will consist of $2dN$ distinct configurations and as all these configurations are included in $|0\rangle$, the state $a_{\mathbf{r}}^\dagger a_{\mathbf{r}+\mathbf{n}}|0\rangle$ will contain $|k\rangle$ with amplitude $2dN$. This amplitude would be $2dN - 2d$ if there had been one vacant site in $|k\rangle$, since now $2d$ jumps from the nearest neighbor sites of the vacant site would be absent. Hence, in general, the amplitude of $|k\rangle$ in $-\mathcal{H}'|0\rangle$ will be $2dN$, and this completes the proof of (i). To prove (ii), let us examine the matrix representation of $-\mathcal{H}'$ in the space of all configurations $|k\rangle$. Each row (or column) will have 1 in $2dN$ places and 0 elsewhere, since $|k\rangle$ is connected to $2dN$ configurations by the Hamiltonian (when there is no vacant site). It follows that the sum of the elements of every row (or column) is $2dN$ which, in view of the

well-known matrix properties [11], is equal to the spectral radius. This completes the proof of (ii).

To calculate now the mass distribution in the ground state, we note that the total number of configurations in $|0\rangle$, i.e., the number of ways in which M bosons can be distributed among N sites (allowing for empty sites) is

$$\Omega_N^M = \binom{M+N-1}{N-1}.$$

This expression is obtained by observing that Ω_N^M is nothing but the coefficient of x^M in the expression $(1+x+x^2+\dots)^N$. As mentioned earlier, $P(m)$ is also the probability $P_{\mathbf{r}}(m)$ of getting m bosons at some particular site \mathbf{r} . Hence, $P(m)$ is simply $1/\Omega_N^M$ times the number of configurations that have m bosons at site \mathbf{r} . This number of configurations is again just the number of ways in which the remaining $M-m$ particles can be distributed among the remaining $N-1$ sites. Therefore, the ground state mass distribution for \mathcal{H}' is, finally,

$$P(m) = \frac{\Omega_{N-1}^{M-m}/\Omega_N^M}{(N-1) \frac{(M+N-m-2)!M!}{(M+N-1)!(M-m)!}}, \quad (8)$$

which, for large M , N , and small m , happens to take the exponential form (7).

Before we conclude, let us compare the mass distributions for the ground states of \mathcal{H} and \mathcal{H}' with the same for the steady state of the classical rule \mathcal{C} . The rule \mathcal{C} is a special case of the model of Majumdar, Krishnamurthy, and Barma [5], with no diffusion and aggregation and only ‘‘chipping’’ present. The mean field equation for this model,

$$\frac{dP(m)}{dt} = [P(0)-2]P(m) + P(m+1) + [1-P(0)]P(m-1),$$

has the same steady-state solution as Eq. (7). We have also checked that the simulation results for \mathcal{C} with 1000 particles also agree with Eq. (7) for reasonable values of density (~ 1 to 10). Thus, the classical distribution resembles the ground state distribution of \mathcal{H}' [Eq. (8)] but not the same of \mathcal{H} [Eq. (6)], as mentioned above. It would be interesting to compare other quantum models with analogous classical models.

Note Added. Mass distribution described by Eq. (7) has been discussed recently in the context of classical models by Majumdar, Krishnamurthy, and Barma [12].

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 [10] See *Nucleation and Growth of Thin Films* (Ref. [6]) pp. 356–365 and 387. The experimental plots there correspond to $m^{2/3}P(m)$ vs $m^{1/3}$ in our language. We have checked that Fig. 1 retains its nature when plotted in this way.
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