Self-Reduction Rate of a Microtubule

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We formulate and study a quantum field theory of a microtubule, a basic element of living cells. Following the quantum theory of consciousness by Hameroff and Penrose, we let the system to reduce to one of the classical states without measurement if certain conditions are satisfied (self-reductions), and calculate the self-reduction time $\tau_N$ (the mean interval between two successive self-reductions) of a cluster consisting of more than $N$ neighboring tubulins (basic units composing a microtubule). $\tau_N$ is interpreted there as an instance of the stream of consciousness. We analyze the dependence of $\tau_N$ upon $N$ and the initial conditions, etc. For relatively large electron hopping amplitude, $\tau_N$ obeys a power law $\tau_N \sim N^b$, which can be explained by the percolation theory. For sufficiently small values of the electron hopping amplitude, $\tau_N$ obeys an exponential law, $\tau_N \sim \exp(cN')$. By using this law, we estimate the condition for $\tau_N$ to take realistic values $\tau_N \gtrsim 10^{-1}$ sec as $N \gtrsim 1000$.

I. INTRODUCTION

Most approaches to understanding various characteristic functions of the human brain in a framework of conventional physics are classical. For example, the Hopfield model of neural network [1], a standard model of associative memory, adopts an Ising spin variable ($\pm 1$) to describe the state of each neuron. In the field of psychophysics, phenomenological relations between psychological quantities (like the sense of pain) and physical quantities (like voltage) in classical physics are of main concern. Although most researchers may agree that the human brain should be described by quantum theory of electrons and atoms at the microscopic level, there seems to be a prejudice that the functions of human brain in our daily life are to be well understood, if possible, by notion of classical physics without recourse to quantum physics.

The problem how to understand mind and consciousness remains as a central and still open question in the physics of the brain. We don’t know even whether the answer to this problem exists. In such a situation, Hameroff and Penrose [2] proposed a quantum theory of consciousness according to a new quantum mechanics of microtubule. Their idea is interesting because it suggests the fundamental importance of quantum measurements and collapses of wave function upon the functions of human brain.

Microtubules are basic building blocks of living cells including neurons and axons, conveying mitochondria, etc. Each microtubule is a hollow cylinder with a diameter $\sim 25$nm, the surface of which is a 2D array of units called tubulins (See Fig.1a). The array consists of 13 columns, and its longitudinal size $L$ is not definite (typically $L = 100 \sim 1000$). Neighboring tubulins in two adjacent columns is displaced with a fixed pitch, so that tubulins form a triangular lattice. A tubulin is a dielectric dimer consisting of an $\alpha$ tubulin monomer and a $\beta$ tubulin monomer.

As a quantum model of a tubulin it is often treated [2-5] as each tubulin contains a single active (mobile) electron and takes two independent states, $|\alpha\rangle$ and $|\beta\rangle$, according to the "upper" or "lower" position of the electron (See Fig.1b). Tuszynski et al. [3] set up and studied some quantum models of a microtubule as a conventional quantum system, i.e., without self-reductions. Also, Rasmussen et al. [4] studied signal propagations along a microtubule by using a network model of cellular automata.

Penrose [5] argued that any quantum system is to be affected through couplings to quantum gravity in such a way that its wave function should make self-reductions (called orchestrated objective reductions) according to certain rules that reflect the uncertainty principle in quantum gravity. In the theory of Hameroff and Penrose [2], a well developed coherent (i.e., superposed) state of each tubulin, $C_\alpha|\alpha\rangle + C_\beta|\beta\rangle$ with $|C_\alpha| \sim |C_\beta|$ has a too large uncertainty of the location of electron, and may be unstable if some other tubulins are also in such states at the same time, from the viewpoint of uncertainty principle of quantum gravity. So each of these tubulins should make a self-reduction to be put back to one of the eigenstates of electron position, $|\alpha\rangle$ or $|\beta\rangle$. They argue that a sequence of such reductions works as a clock and forms a stream of consciousness. The mean time between two successive reductions, which we call the self-reduction time $\tau$, is interpreted as each moment of consciousness.

Then quantitative estimation of $\tau$ would become a main concern. However, tegmark [6] posed a question that a microtubule suffers from decoherence effects through quantum interactions with its environment, for instance ions and water molecules in the surrounding cytoplasm, and the decoherence time $\tau_{\text{dec}}$ (the time scale to lose off-diagonal elements of the reduced density matrix, hence to destroy long-range quantum superpositions) may be much smaller than the self-reduction time $\tau$. If this is true, the scenario by Hameroff and Penrose loses its reality. He estimated the decoherence time $\tau_{\text{dec}}$ of an entire microtubule at finite temperatures as $\tau_{\text{dec}} \lesssim 10^{-6}$...
10^{-13} \text{ sec} and claimed that microtubules can be treated classically in the interesting time scales $10^{-1} \sim 10^{-2} \text{ sec}$ for a stream of consciousness, and quantum effects play no significant role there. Then Hagan et al. [7] responded for a stream of consciousness, and quantum effects play no significant role there. Then Hagan et al. [7] responded for a stream of consciousness, and quantum effects play no significant role there.

In this paper we leave this problem of estimating the decoherence time as a still controversial and open problem, and concentrate on the quantitative estimation of the self-reduction time $\tau$ itself of an isolated microtubule at zero temperature without external disturbances, thus ignoring decoherence effect by the environment. An ensemble of microtubules and/or the effects of temperature and environment [6,7] should be considered in the next step. Explicitly, we set up a quantum theory based on the classical model of Rasmussen et al. [4] and calculate $\tau$ by proposing some rules of self-reductions based on the Hameroff-Penrose theory. Such a study should certainly present some important informations to scrutinize the relevance of Hameroff-Penrose theory. Since the typical time scale set by the Coulomb energy at nano scales is $\sim 10^{-15} \text{ sec}$, the central question is whether $\tau$ can take values of the order of $10^{-1} \sim 10^{-2} \text{ sec}$ which seems to be reasonable as the moment of consciousness. We shall see that $\tau$ exhibits systematic behaviors which may be typical for models of self-reductions.

One may conceive reasons of self-reductions other than Penrose’s proposal based on quantum gravity [5]. Ghi rard et al. [8] propose a modification of Schrödinger equation to a nonlinear stochastic equation to incorporate dynamical reductions. As yet another possibility, (quasi)reductions may occur due to internal quantum measurements of microtubule by surrounding environment in the brain, or even the microtubule itself may “measure” its part [9]. Our rules of self-reductions are phenomenological and may mimic these cases.

The rest of the paper is organized as follows: In Sect.2 we set up a quantum field theory of a microtubule. It may be interpreted as a frustrated quantum spin model in two dimensions. We propose to study its dynamics by solving an approximate Schrödinger equation derived by the variational method. In Sect.3 we calculate the self-reduction time $\tau_N$ for various conditions. We find that $\tau_N$ exhibits different behaviors depending whether the electron hopping amplitude is large or small. In Sect.4 we present conclusion.

II. MODEL

A. Hamiltonian

The Hamiltonian $H$ of a microtubule is given by

$$H = -k \sum_i \sum_{\gamma=\alpha,\beta} b_i^\dagger \gamma b_i \gamma + \sum_{(i,j)} V^\gamma_{ij} b_i^\dagger \gamma b_j \gamma,$$

where $\alpha \equiv \beta, \bar{\beta} \equiv \alpha$. $b_i \gamma, b_i^\dagger \gamma (\gamma = \alpha, \beta)$ are the fermionic annihilation and creation operators of the electron in the $\gamma$ state at the $i$-th tubulin, satisfying

$$[b_i \gamma, b_j^{\dagger \gamma}]_+ = 0, \quad [b_i \gamma, b_j^{\dagger \gamma}]_+ = \delta_{ij} \delta_{\gamma \gamma'}.$$

$\epsilon$ is a dielectric constant of the microtubule. The first term of $H$ represents the kinetic energy of the electron changing its state $\alpha \leftrightarrow \beta$ within the $i$-th tubulin with the hopping amplitude $k$. The second term represents the Coulomb energy $V^\gamma_{ij}$ between two electrons at $(i \gamma)$ and $(j \gamma')$ separated by the distance $R^\gamma_{ij}$, the value of which is given in Ref. [4]. $\sum_{(i,j)}$ implies the sum over all the neighboring pairs $i,j$ given in Fig.1 (Each tubulin has six neighbors). The number of electrons in each tubulin is a constant of motion,

$$N_i \equiv \sum_{\gamma} b_i^\dagger \gamma b_i \gamma, \quad [H, N_i] = 0. \quad (2.3)$$

In actual calculations, we start and stay in the subspace $N_i = 1$.

This Hamiltonian may be expressed in terms of the $s = 1/2$ SU(2) quantum spin operator $\vec{S}_i \equiv (\hbar/2)(b_{i\alpha}^\dagger b_{i\beta} + b_{i\beta}^\dagger b_{i\alpha})\vec{\sigma}$ ($\vec{\sigma}$ are Pauli matrices) as

$$H = -\sum_{(i,j)} J_{ij} S_{iz} S_{jz} - \sum_i \vec{B} \cdot \vec{S}_i + \text{const}, \quad (2.4)$$

with

$$J_{ij} = -\frac{1}{\hbar^2} \left(V^{\alpha \alpha}_{ij} - V^{\alpha \beta}_{ij} - V^{\beta \alpha}_{ij} + V^{\beta \beta}_{ij}\right),$$

$$B_x = \frac{2k}{\hbar}, \quad B_y = 0,$$

$$B_z = -\frac{1}{2\hbar} \sum_{j(\text{NN to } i)} \left(V^{\alpha \alpha}_{ij} + V^{\alpha \beta}_{ij} - V^{\beta \alpha}_{ij} - V^{\beta \beta}_{ij}\right) = 0. \quad (2.5)$$
The values of \( J_{ij} \) are

\[
\begin{align*}
J_{\text{North}} &= J_{\text{South}} = 0.0833h^{-2}V_0, \\
J_{\text{SE}} &= J_{\text{NW}} = 0.0091h^{-2}V_0, \\
J_{\text{NE}} &= J_{\text{SW}} = -0.0280h^{-2}V_0, \\
V_0 &= \frac{1}{\epsilon} \cdot \frac{e^2}{1\text{nm}} = \frac{1}{\epsilon} \cdot 2.31 \times 10^{-19}\text{Joule},
\end{align*}
\]

where \( V_0 \) is the Coulomb energy of a pair of electrons in the microtubule separated by 1 nm. So the system may be viewed as a frustrated spin model in an external magnetic field \( \vec{B} \). At \( k = 0 \), the system involves only \( S_z \), and its ground state is found to be the “stripe state” in which \( S_z \) are aligned to \( \pm \hbar/2 \) along each column with the alternative signs, except for a pair of two NN columns (1st and 13th, say) with the same signs. The degeneracy is \( 13 \times 2 \) [10]. As \( k \) increases, the \( S_z \) component develops, and at \( k \to \infty \), all \( S_i \) align to \( (\hbar/2)(1,0,0) \).

### B. Time evolution in variational method

In the time interval between two successive self-reductions, the state vector \( |\psi(t)\rangle \) of a microtubule at time \( t \) evolves according to the Schrödinger equation,

\[
i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle.
\]

If the microtubule contains \( V \) tubulins, then \( |\psi(t)\rangle \) is \( 2^V \) dimensional, and for \( V \gtrsim 13 \times 100 \), the precise evaluation of \( |\psi(t)\rangle \) is beyond the ability of our computers. Thus, we evaluate \( |\psi(t)\rangle \) approximately by the variational method. Explicitly, we choose the variational state \( |\psi_v(t)\rangle \) in the factorized form,

\[
|\psi_v(t)\rangle = \prod_i \left[ C_{i\alpha}(t) |i\alpha\rangle + C_{i\beta}(t) |i\beta\rangle \right],
\]

\[
|C_{i\alpha}(t)|^2 + |C_{i\beta}(t)|^2 = 1,
\]

where

\[
|i\gamma\rangle \equiv b_{i\gamma}^\dagger |0\rangle_i, \quad b_{i\gamma}|0\rangle_i = 0,
\]

is the state of the \( i \)-th tubulin in which the electron is in the \( \gamma \) state. By minimizing the action,

\[
S = \int_{t_1}^{t_2} dt \langle \psi_v(t)| \left( i\hbar \frac{d}{dt} - H \right) |\psi_v(t)\rangle,
\]

we get the following equations of motion for \( 2V \) complex coefficients \( C_{i\gamma} \):

\[
i\hbar \frac{dC_{i\gamma}}{dt} = -kC_{i\bar{\gamma}} + J_{i\gamma}C_{i\gamma},
\]

\[
J_{i\gamma} = \sum_{j \text{(NN to } i)} \left( V_{ij}^\alpha C_j\alpha|^2 + V_{ij}^\beta C_j\beta|^2 \right).
\]

Eq.(2.5) respects the unitarity,

\[
|C_{i\alpha}(t)|^2 + |C_{i\beta}(t)|^2 = 1,
\]

and keeps the average \( E_v \equiv \langle \psi_v(t)|H|\psi_v(t)\rangle \) a constant of motion.

We note that, if \( \Delta V_{ij}^\gamma \equiv V_{ij}^\alpha - V_{ij}^\beta \) is negligible,

\[
J_{i\gamma} \approx \frac{1}{2} \sum_j (V_{ij}^\alpha + V_{ij}^\beta) \equiv \bar{J}
\]

becomes independent of neighboring \( C_{j\beta} \)'s, so Eq.(2.5) are decoupled to give the mean-field solution (MFS),

\[
C_{i\alpha}(t) = C_i + e^{-i\Omega t} + (-)e^{i\Omega t},
\]

\[
C_{i\beta}(t) = \frac{1}{2} |C_{i\alpha}(0) \pm C_{i\beta}(0)|, \quad \Omega = \bar{J} + k.
\]

The actual value of \( |\Delta V_{ij}^\gamma|/(V_{ij}^\alpha + V_{ij}^\beta) \) averaged over \( j \) is 0.19, so the couplings between neighboring tubulins are intermediate.

We solve the differential equations (2.5) numerically by the Runge-Kutta method with discrete time step \( \Delta t \). As the initial condition \( C_{i\gamma}(0) \) at \( t = 0 \), we consider the following four cases:

(i) US(Uniform Start); \( C_{i\alpha}(0) = 1, C_{i\beta} = 0 \) for all \( i \),

(ii) SS(Stripe Start); \( C_{i\alpha}(0) = 1, 0 \) for alternative columns as explained,

(iii) RIS(Random Ising Start); \( C_{i\gamma}(0) = 1, 0 \), randomly,

(iv) RCS(Random complex Start); \( C_{i\gamma}(0) \in C \) randomly.

### C. Rule of self-reductions

For the rule of self-reductions, we follow the idea of Hameroff and Penrose [2]. We first choose a parameter \( P_0 \) and prepare the “reset zone” of \( C_{i\alpha}(t) \),

\[
P_0 \leq |C_{i\alpha}(t)|^2 \leq P_1 (\equiv 1 - P_0).
\]

When \( C_{i\alpha}(t) \) is in this zone, we judge that the state \( |i\alpha\rangle \) is sufficiently coherent and may need a self-reduction. In the simulation we watch whether \( |C_{i\alpha}(t)|^2 \) falls into this zone at every time step. The tubulins that are in the reset zone form a cluster, a set of tubulins that are connected each other as neighboring pairs. If the size of cluster at \( t = t_R \) is same or more than the prefixed number \( N \), we let all tubulins within this cluster make self-reductions at the next time step. As the rule to determine \( C_{i\gamma}(t_R + \Delta t) \), we consider the following two cases:

**LR** : Local reduction; Each tubulin reduces to \( |i\alpha\rangle \) or \( |i\beta\rangle \) according to the probabilities \( |C_{i\gamma}(t_R)|^2 \).

**GR** : Global reduction; All the tubulins in the cluster reduce to the common state, \( |\gamma\rangle \), with the probabilities \( |\langle C_{\gamma R}(t) \rangle|^2 \), the averages over the cluster.
In Fig. 2 we show typical time dependence of $|C_{a0}(t)|^2$ for two values of $k$. For larger $k$ the smooth motion between reductions is rather regular, reaching the endpoints 0 and 1 at every period. For smaller $k$, the motion between reductions is often pulled back before reaching the endpoints. This difference is explained as the effect of potential term in $H$ (See Sect.IIIa and IIIb).

In Fig. 3 we show typical snapshots of $|C_{a0}(t)|^2$ for a part of a microtubule before and after a reduction.

To calculate the self-reduction time $\tau_N$ for the minimum cluster size $N$, we make a sufficiently long run with the period $t_{\text{total}}$ for each $N$. $\tau_N$ is then defined as

$$\tau_N = \lim_{t_{\text{total}} \to \infty} \frac{t_{\text{total}}}{M_N},$$

(2.10)

where $M_N$ is the total number of all the self-reductions within the run. So $\tau_N$ is the average time interval between two successive reductions. $\tau_N$ may be expressed by using the probability $p_N$ that clusters of size equal to or larger than $N$ appear as

$$\tau_N \propto \sum_{m=1}^{\infty} m(1-p_N)^{m-1}p_N = \frac{1}{p_N},$$

(2.11)

In the simulations we consider microtubules of the length $L$ up to $L = 2000$ (16 $\mu$m) with the open boundary condition. We choose

$$\Delta t = 0.01 \times t_0,$$

$$t_0 \equiv \frac{\hbar^2}{V_0} = \frac{\hbar \epsilon \times 1 \text{nm}}{e^2} = 4.571 \times 10^{-16} \times \epsilon \text{ sec},$$

(2.12)

where $t_0$ is the time scale set by the Coulomb energy $V_0$ at 1 nm. We choose sufficiently large $t_{\text{total}}$ up to

$$t_{\text{total}} = 2 \times 10^6 \text{ steps} \times \Delta t,$$

(2.13)

to obtain stable values of $\tau_N$. The above $\Delta t$ is checked to be sufficiently small for this $t_{\text{total}}$. To determine the clusters at each $t$, we adopt the algorithm of Hoshen and Kopelman [11] developed in percolation theory [12]. In Table 1 we collect the parameters and their values used in our simulations.

| parameter     | symbol | value                  |
|---------------|--------|------------------------|
| hopping       | $k$    | 0.002 $\sim 2(\times V_0)$ |
| amplitude     |        |                        |
| length        | $L$    | 50 $\sim 2000$         |
| initial stripe (SS) |        | All                    |
| condition     | random Ising (RIS) |                       |
| random complex (RCS) |        |                       |
| cluster size  | $N$    | 5 $\sim 20000$         |
| reset zone    | $P_0$  | 0.01 $\sim 0.49$       |
| reduction     | global reduction (GR) |                     |
| condition     | local reduction (LR) | both                  |
| elapsed time  | $t_{\text{total}}$ | $10^6 \sim 2 \times 10^6(\times t_0)$ |

Table 1. Parameters used in simulation.

We note that the Schrödinger equation (2.1) is invariant under $t \to \lambda t$ and $H \to \lambda^{-1}H$. This is reflected also in the equation of motion (2.5). Thus, $\tau$ is proportional to the dielectric constant $\epsilon$ when $k$ is measured in unit of $V_0$. Experimental measurements of $\epsilon$ are still not definitive but predict values like $\epsilon = 8.41$ [13], $1 < \epsilon < 100$ [14], etc. Also, if the charge of the mobile object which determines the tubulin state, $|\alpha\rangle$ or $|\beta\rangle$, is modified from $-e$ of a single electron to $-ne$, its effect is to be reflected by replacing $\epsilon \to \epsilon/n^2$ in the formulae below.

III. SELF-REDUCTION TIME

As we shall see, $\tau_N$ exhibits different $N$ dependences for large $k$’s and small $k$’s. We study the case of large $k$ first, and then the case of small $k$.

A. Large hopping amplitude $k$

Let us first consider the case of large $k$. In Fig. 4 we plot $\tau_N$ vs. $N$ for $k = 0.1V_0$ for several values of $P_0$. For all the four initial conditions, $\tau_N$ up to $N \lesssim V/2$ can be fitted well by the power law,
is given by

\[ p \propto N \times t_0, \]

\[ a \simeq 1.02 \times 10^{-3} t_0, \quad b \simeq 1.08 \quad \text{for} \quad P_0 = 0.3. \]  

(3.1)

Eq.(3.1) may be explained by adopting the independent oscillator model where \( |C_{\alpha}(t)|^2 \) is given by (2.8). Then the probability \( p \) that each \( |C_{\alpha}(t)|^2 \) is in the reset zone is given by

\[ p = 1 - \frac{2}{\pi} \cos^{-1}(1 - 2P_0). \]

(3.2)

For \( P_0 \geq 0.146 \), \( p \) is below the critical probability \( p_c = 0.5 \) of the triangular lattice above which percolation takes place [12]. The scaling argument [12] predicts \( P_N \) for \( p < p_c \) as

\[ P_N \propto \sum_{s=N}^{\infty} s^{-\delta} f(z) \propto \left\{ \begin{array}{ll}
N^{-\delta+1}, & (p_c - p)N^\sigma \lesssim 1, \\
\epsilon^{-cN}, & (p_c - p)N^\sigma \gtrsim 1,
\end{array} \right. \]

(3.3)

where \( f(z), z \equiv (p_c - p)s^\alpha \), is the scaling function and the exponents are given by [12]

\[ \delta = \frac{187}{91}, \quad \sigma = \frac{36}{91}, \quad c \propto (p_c - p)^{1/\sigma}. \]

(3.4)

By assuming

\[ (p_c - p)N^\sigma \lesssim 1, \]

(3.5)

\[ \tau_N \propto \frac{1}{P_N} \propto N^{\delta-1} \]

giving us the form of (3.1) with

\[ b = \delta - 1 = 1.055. \]

(3.6)

For \( N \gtrsim V/2 \), only one large cluster is possible and all the tubulins in it exhibit a synchronized (collective) motion as

\[ |C_{\alpha}|^2 \simeq \rho_{\text{sync}}(t) \equiv \cos^2 \left( \frac{k}{\hbar} (t - t_R) \right) \text{ or } \sin^2 \left( \frac{k}{\hbar} (t - t_R) \right), \]

\[ \tau_N \simeq \tau_{\text{sync}} \equiv \frac{\hbar}{2k} \times \cos^{-1}(1 - 2P_0), \]

(3.7)

as the MFS (2.8) predicts. In fact, Fig.4 shows that \( \tau_N \) saturates to \( \tau_{\text{sync}} \) for \( N \gtrsim V/2 \). Thus \( k = 0.1 V_0 \) is “large”, where the coupling to neighbors via \( \Delta V_{ij} \) is negligible. Here the system is in the single-body regime.

B. Small hopping amplitude \( k \)

Let us next consider the case of small \( k \)’s. For small \( k \)’s, \( \Delta V_{ij} \) becomes relevant. In Fig.5 we plot \( \tau_N \) vs. \( N \) at \( k = 0.01 V_0 \). Here each \( |C_{\alpha}(t)|^2 \) basically sweeps between 0 and 1 with a basic frequency \( \sim k/\hbar \), but is sometimes “pulled back” due to \( \Delta V_{ij} \) (See Fig.2b). The system is in the many-body regime where the potential term is relevant. As \( N \) increases, \( \tau_N \) in Fig.5 exhibits a crossover from the power law to the exponential law. We note that, although the tubulins are not independent each other as here explained, Eq.(3.3) may describe this crossover phenomenologically (with an effective \( p_c - p \), etc.). The exponential behavior of Fig.5 is fitted as

\[ \tau_N \simeq a' \exp(c'N), \]

\[ a' \simeq (0.40 \sim 1.30) \times 10^{-14} \times \epsilon \sec, \]

\[ c' \simeq 0.025 \sim 0.029 \quad \text{for} \quad P_0 = 0.3, L = 50 \sim 200. \]

(3.8)

To study the condition for \( \tau_N \) to take realistic values, extremely long runs are required. So let us assume (3.8) to hold for larger \( N \)’s as an asymptotic expression, and extrapolate it to estimate the minimum size \( N \) of the cluster. For \( k = 0.01 V_0 \), \( P_0 = 0.3 \) and \( a' = 0.85 \times 10^{-14} \times \epsilon \sec \), \( c' = 0.027 \) we obtain the minimum \( N \) for typical values of the dielectric constant \( \epsilon \) in Table 2 below.

| \( \tau \geq 10^{-2} \sec \) | \( \tau \geq 10^{-1} \sec \) |
|---|---|
| \( \epsilon = 1 \) | \( N \geq 1030 \) | \( N \geq 1115 \) |
| \( \epsilon = 10 \) | \( N \geq 945 \) | \( N \geq 1030 \) |
| \( \epsilon = 100 \) | \( N \geq 860 \) | \( N \geq 945 \) |

Table 2. Minimum size of the cluster for \( \tau > 10^{-2} \sec \), \( 10^{-1} \sec \) and various \( \epsilon \) at \( k = 0.01 V_0 \) and \( P_0 = 0.3 \) calculated by Eq.(3.8).

FIG. 5. \( \tau_N \) vs. \( N \) for \( k = 0.01 V_0 \) with RIS/LR. \( \tau_N \) exhibits a crossover from the power law (\( \propto N^{b'} \), \( b' \simeq 1.56 \) for \( P_0 = 0.3 \); dashed curves) to the exponential law (3.8) (dashed straight lines).
C. $k$-dependence and the estimation of $k$

Let us study the $k$-dependence of $\tau_N$ in detail. In Fig.6 we plot $\tau_N$ vs. $k$ for $N = 0.1V$ and $N = V$ with $L = 200, P_0 = 0.3$ and LR. Let us first consider $N = V$. Simulations with RCS show no reductions throughout runs due to the random initial configurations. For the other three initial conditions, the data (in black) at large $k$'s lie on the line $\tau_N = \tau_{\text{sync}} (3.7)$ of the synchronized behavior of single cluster explained for Fig.4. As $k$ decreases, they deviate from $\tau_{\text{sync}}$ suddenly at the point marked as $a$ with $k = k_a \approx 0.07V_0$ As $k \rightarrow 0$, $\tau_N$ blows up. This is because these SS, US, and RIS become exact eigenstates of $H$ at $k = 0$; each initial eigenstate has time-independent $|C_{\alpha}(t)|^2 (= 0, 1)$, hence no reductions are possible. Let us next consider $N = 0.1V$. The SS, US, and RIS data start from $\tau_{\text{sync}}$ at large $k$ and deviate from it downward at the point $b$ and join the RCS data. They start to blow up at $c$. The decrease of $\tau_N$ at $b$ reflects generations of plural clusters.

In Fig.7 we plot $\tau_N$ vs. $k$ for various values of $P_0$ with RIS/LR, $N = V/2, L = 200$. The data show systematic dependence on $P_0$. As $P_0$ increases, the reset zone becomes narrow and $\tau_N$ at fixed $k$ increases. The point of blowing up, $k = k_a$, also increases as $P_0$.

In Fig.8 we plot an interpolating curve of $k_a$ in Fig.7 as a function of $P_0$. It separates two regimes: (i) single-body regime for $k > k_a$ where the kinetic term in $H$ dominates over the potential term and the dynamics of each tubulin is well described by the synchronized motion of Eq.(3.7) and (ii) many-body regime for $k < k_a$ where the potential term dominates over the kinetic term. As Figs.6,7 show, the change between these two regimes is very sharp.

Let us estimate the value of $k$. For this purpose, we assume a hydrogen-like wave function for $|\alpha\rangle$ and $|\beta\rangle$ states:

$$\langle \vec{r}\gamma \rangle \propto \exp(-\frac{|\vec{r}-\vec{r}_0|}{\ell})$$

Then, by a straightforward calculation, one obtains

$$k \simeq \frac{\langle \alpha | e^{2\gamma} | \beta \rangle - \langle \alpha | \beta \rangle \langle \alpha | e^{2\gamma} | \alpha \rangle}{\epsilon (1 - \langle \alpha | \beta \rangle^2)}. \quad (3.10)$$

In Fig.9 we present $k$ vs. $\ell$ calculated from Eq.(3.10) by putting $|\vec{r}_0 - \vec{r}_\beta| = 4$nm as shown in Fig.1b. It seems that the reasonable value of $k$ may be within the range $0.01V_0 \lesssim k \lesssim 0.1V_0$.
For $\tau_{\text{con}}$, it is reasonable to estimate as $\tau_{\text{con}} \approx 10^{-1} \sim 10^{-2}$ sec. Then the exponential law (3.8) for $\tau_{N}$ at small $k$ shows that, in order to satisfy the second inequality of (4.1), one needs $N > 1000$ as Table 2 shows. This cluster size is realistic enough, because it is the same order or smaller than the typical size of microtubule, $V = (100 \sim 1000) \times 13$, explained in Sect.1. Thus, our present analysis shows that the second inequality holds. Concerning to the first inequality of (4.1), estimation of $\tau_{\text{dec}}$ is crucial, but, as stated in Sect.1, it is still controversial [6, 7]. We need reliable estimation of $\tau_{\text{dec}}$. Here we point out that a possible quantum ordered state of a microtubule or a set of microtubules with spontaneous symmetry breaking and an off-diagonal long-range order may give rise to an extra stability of coherence against decoherent fluctuations due to the environment, leading to much larger values of $\tau_{\text{dec}}$. This possibility is pointed out by Penrose [5] and others in a general point of view. Because there is now an explicit quantum model (2.1), one may explore such possibility in a quantitative manner using conventional techniques of quantum field theory and statistical mechanics. This is certainly an interesting future problem.

In conclusion, we set up a quantum field theory of microtubule and estimated the self-reduction time $\tau_{N}$. $\tau_{N}$ exhibits systematic behaviors; the power law in the single-body regime for $k > k_{a}$, or the exponential law in the many-body regime for $k < k_{a}$. $\tau_{N}$ can take arbitrary large values if one imposes unrealistic conditions like $k \rightarrow 0$, $N \rightarrow \infty$, or $P_{0} \rightarrow 0.5$. Further experimental studies of microtubules, e.g., determination of $k$, may lead us to better understanding of their behaviors; We may then be ready to answer some interesting questions like whether they are sitting on “the edge of chaos” discussed in the study of complex systems [15].

Concerning to the approximation(variational method), we point out a possibility that the approximate solution plus self-reductions as we imposed may mimic the exact solutions of Schrödinger equation. Then we do not need extra coupling to quantum gravity claimed by Penrose. It is interesting to investigate whether the conventional quantum theory itself exhibits (quasi)reductions by letting its subsystems make self-(quasi)reductions [9].

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