Mössbauer effect as a possible tool in detecting nonlinear excitations in microtubules

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We investigate the electronic degrees of freedom in cytoskeletal microtubules in the continuum approximation. The equations of motion of the propagating local conformational state are solved in the low temperature regime. The solution, which is a kink excitation, is coupled to the motion of the mobile electron of the constituent tubulin. We calculate the influence of kink excitations on the probability of the Mössbauer emission of γ-active nuclei. A discussion follows on this potentially useful experimental tool for the detection of nonlinear excitations in a microtubule. [S1063-651X(98)14810-9]

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I. INTRODUCTION

Microtubules have recently attracted considerable attention from physicists as very important biological structures [1] characterized by a substantial amount of symmetry, regularity, and rigidity [2]. Microtubules (MT's) are long polymers formed from globular tubulin protein dimers which are found in abundance in all types of eukaryotic cells. MT's can be described as long, hollow cylinders composed of (typically) 13 protofilaments aligned along the MT axis (see Fig. 1). A requisite structural element in all MT's appears to be a vertical seam, resulting in a so called *B*-type lattice [3]. Each constituent tubulin subunit is a polar, 8-nm-long dimer which consists of two slightly different 4-nm monomers, each of which has a molecular weight on the order of 55 kilodaltons. The two monomers comprising a structural dimer unit are often referred to as α- and β-tubulin.

Tubulin dimers are known to possess a permanent dipole moment due to a mobile electron which may be localized either in the α or β tubulin region (see Fig. 2). In the latter case, a local conformational change is associated with the electron's tunneling, and hence indicates the existence of piezoelectric properties. MT's exhibit fascinating assembly and disassembly phenomena present both *in vivo* and *in vitro* [3,4], whose elucidation is another challenging task for both biologists and physicists. Furthermore, MT's have been identified as likely candidates for information processing and signaling effects at a subcellular level [5–7]. Recently, two groups independently proposed models of MT dynamics based on nonlinear kinklike excitations propagating along each protofilament [8,9]. The conceptual basis for the model developed in Ref. [8] is the classical ϕ^4 theory, which is generic for systems undergoing second-order phase transitions. It was demonstrated in Ref. [8] that kinklike excitations may arise as a result of the GTP→GDP hydrolysis which seems to accompany the process of MT assembly. The intrinsic electric field along the protofilament axis may cause kinks to propagate down the MT, thereby transporting energy from the lateral cap [10] at the distal tip to the opposite end of a MT in the course of assembly. The above hypothesis must still be verified experimentally, and in this paper we suggest the Mössbauer effect as an appropriate tool. It was recently described how the Mössbauer effect may be used to detect the presence of nonlinear excitations in anharmonic chains [11,12]. In the present paper we intend to apply this idea to the case of microtubules. This requires the use of radioactive nuclei which can be built into the MT structure. We will assume such a possibility, and carry out calculations

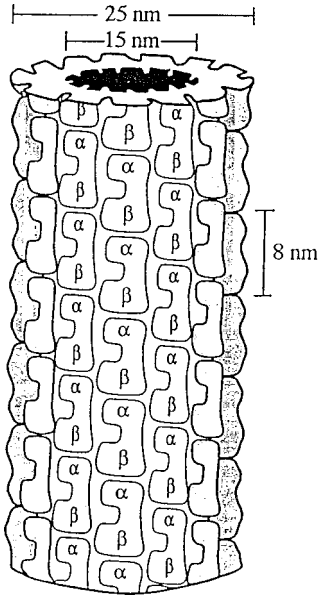

FIG. 1. A schematic diagram of a microtubular structure.

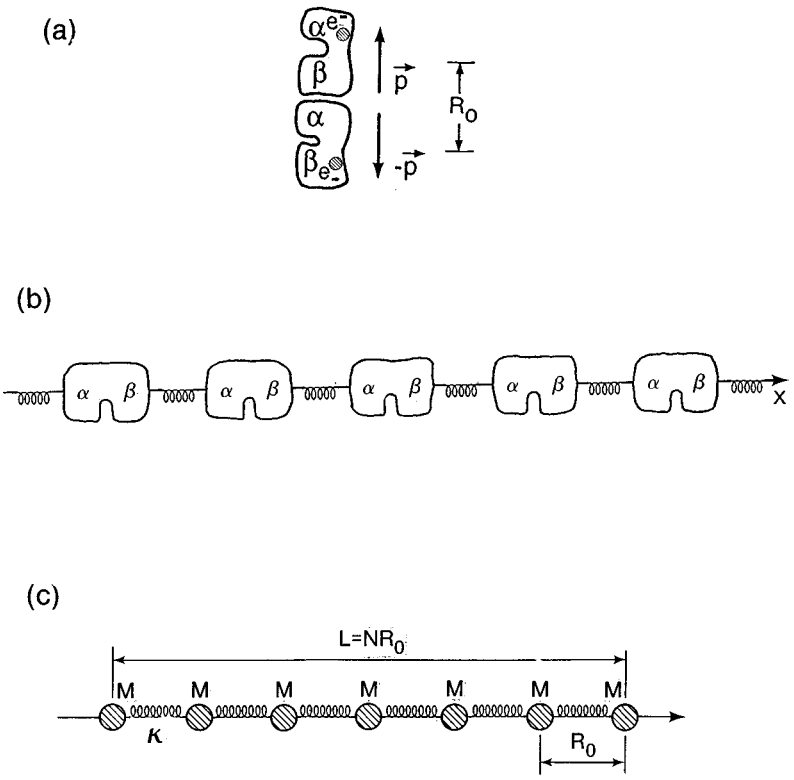

FIG. 2. The two electronic states of a tubulin dimer.

which account for the coexistence of both quantum phonon modes and classical nonlinear kinklike excitations. Before we present these results, however, it is necessary to present the physical model in more detail.

II. PHYSICAL MODEL

An important conclusion can be drawn from recent Monte Carlo simulations of dipole dynamics in microtubules, namely, that, close to the transition temperature T_c, the system can be adequately described in terms of one order parameter, i.e., the net polarization along the protofilament axis, denoted by $P \equiv \langle P_z \rangle$. The displacement of the monomer at site n is denoted by u_n, and must be related with P_n by the simple equality $P_n = q u_n$, where q represents the effective mobile charge of the monomer. Since the transition studied is obviously of second order we may, in the regime of sufficiently long MT's, involve a continuum approximation with the effective Hamiltonian of the form

$$H_{\text{eff}} = \int dx \left[-\frac{1}{2} A u^2 + \frac{1}{4} B u^4 - qEu + \frac{k}{2} \left(\frac{\partial u}{\partial x} \right)^2 + \frac{M}{2} \left(\frac{\partial u}{\partial t} \right)^2 \right] \tag{2.1}$$

where $A = a(T - T_c)$, $B > 0$ and $E = E_0 + E_{\text{ext}}$. Here E_0 is an intrinsic electric field due to the anisotropy of the microtubule, while E_{ext} is an externally applied electric field. The effective potential

$$V_{\text{eff}} = -\tfrac{1}{2} A u^2 + \tfrac{1}{4} B u^4 - Equ \tag{2.2}$$

is shown in Fig. 3 for both $T > T_c$ and $T < T_c$, as well as in several cases of E.

The coefficient k arises in the continuum limit of the nearest-neighbor dipole-dipole interaction $\mathcal{I}$ in accordance with the expansion

$$\mathcal{I} d_i d_{i \pm 1} = \mathcal{I} d_i^2 - \mathcal{I} R_0^2 (\nabla d)^2 + \cdots ,$$

where R_0 represents the equilibrium distance between neighboring dimers with their corresponding dipole moments d_i and $d_{i \pm 1}$.

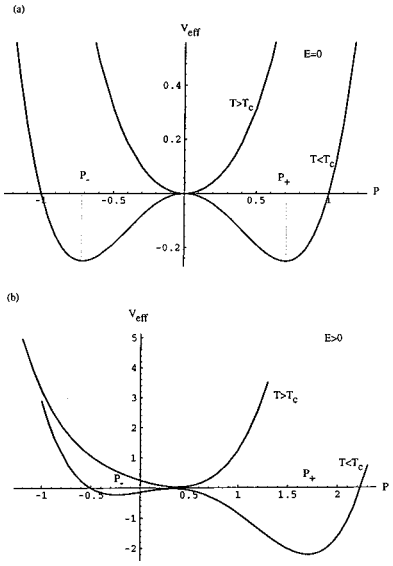

FIG. 3. The various possible shapes of the effective potential above and below the critical temperature. The axes are plotted in arbitrary units.

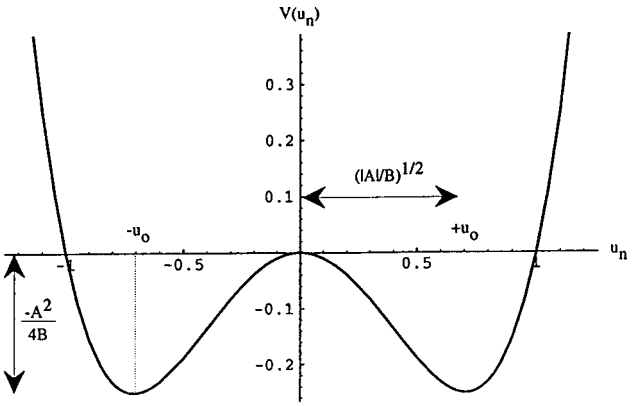

FIG. 4. The symmetric double-well potential of Eq. (2.5). The axes are plotted in arbitrary units.

The potential V_{eff} accounts for the onset of long-range order equilibrium in the near-critical regime. At equilibrium it holds that

$$\frac{\partial V_{\text{eff}}}{\partial u} = -Au + Bu^3 - qE = 0. \tag{2.3}$$

The effect of E_0 may be indirectly linked to the well-documented [13] presence of the so-called clear zone which is a region of several ionic distances surrounding a MT. This serves, as a buffer between the MT and other structures (including other MT's) floating in the cytoplasm, and it is believed to originate in the intrinsic electric field produced by a MT. In order to account for the fact that dipolar states are coupled to a local conformational state, the model Hamiltonian should contain a kinetic energy term responsible for oscillatory dynamics around equilibrium. The coefficient M represents the effective mass of the moving monomer.

In order to derive a realistic equation of motion for the system described above, it is necessary to include the viscosity of the solvent and introduce the associated damping force. Assuming, for simplicity, that the solvent is made up of only water molecules, the viscosity can be simply taken into account by adding a friction force to the equation of motion with

$$F_v = -\gamma \frac{du_n}{dt}, \tag{2.4}$$

where γ represents the damping coefficient. An equation of motion for dipolar oscillations can be thus derived using the Hamiltonian of Eq. (2.1), applying the continuum limit, and adding the viscous force of Eq. (2.4). As a result [8], one obtains

$$\frac{d^2Y}{d\xi^2} + \rho \frac{dY}{d\xi} - Y^3 + Y + \sigma = 0, \tag{2.5}$$

where $Y(\xi)$ represents the normalized displacement field $Y(\xi) = u(\xi)/u_0$, where $u_0 = (|A|/B)^{1/2}$ corresponds to the minimum of the double-well potential (Fig. 4). The independent variable ξ is the moving coordinate for the traveling-wave form of the solution, i.e.,

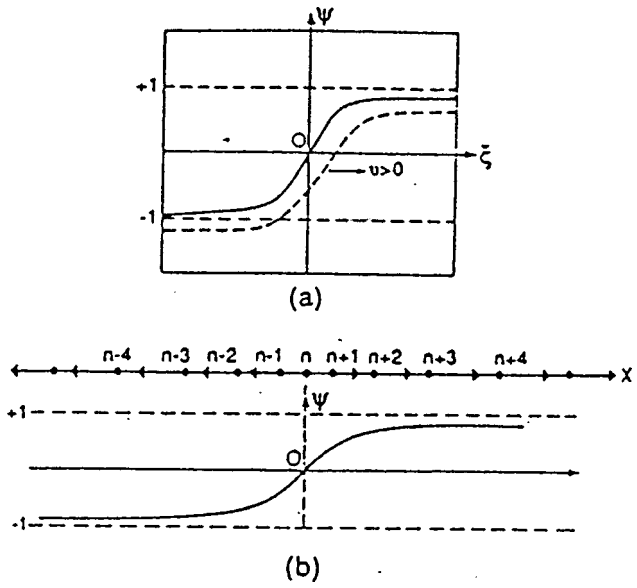

FIG. 5. The kink solution of Eq. (2.9). The axes are plotted in arbitrary units.

$$\xi = \left(\frac{|A|}{M(v_0^2 - v^2)}\right)^{1/2} (x - vt) = \alpha(x - vt),$$

$$\alpha = \left(\frac{|A|}{M(v_0^2 - v^2)}\right)^{1/2}, \tag{2.6}$$

where v denotes the propagation velocity for the dipolar mode, while $v_0 = R_0(k/M)^{1/2}$ represents the longitudinal sound velocity through the MT. The remaining parameters of Eq. (2.5) are

$$\rho = \gamma v [M(v_0^2 - v^2)/|A|]^{-1/2} \tag{2.7}$$

and

$$\sigma = q\sqrt{B}A^{-3/2}E. \tag{2.8}$$

It can be shown that Eq. (2.5) has a unique bounded solution which gives, for the displacement field, the formula

$$u(\xi) = u_2 + \frac{u_1 - u_2}{1 + \exp[\delta(u_1 - u_2)\xi]}, \tag{2.9}$$

which is illustrated graphically in Fig. 5, and where

$$u_1 = 2\left(\frac{A}{3B}\right)^{1/2} \cos\left\{\frac{1}{3}\arccos\left[\frac{3qE}{2A}\left(\frac{3B}{A}\right)^{1/2}\right]\right\},$$

$$u_2 = -2\left(\frac{A}{3B}\right)^{1/2} \cos\left\{\frac{\pi}{3} - \frac{1}{3}\arccos\left[\frac{3qE}{2A}\left(\frac{3B}{A}\right)^{1/2}\right]\right\},$$

$$\delta = \pm\frac{1}{v_0}\left(\frac{B}{2M}\right)^{1/2}. \tag{2.10}$$

Thus solution (2.9) is a kink solution giving the boundary between the two asymptotic states $u = u_1$ for $\xi \to +\infty$ and $u = u_2$ for $\xi \to \infty$, if $\delta > 0$.

The boundary moves with the unique terminal velocity

$$v=\pm\frac{v_0}{\gamma}\left(\frac{6A}{M}\right)^{1/2}\cos\left\{\frac{\pi}{3}+\frac{1}{3}\arccos\left[\frac{3qE}{2A}\left(\frac{3B}{A}\right)^{1/2}\right]\right\}, \tag{2.11}$$

and its width Δ is given by

$$\Delta=\frac{v_0}{u_1-u_2}\left(\frac{2M}{B}\right)^{1/2}. \tag{2.12}$$

It is important to make an estimate of the above quantities. For a long MT we can assume that for points that are sufficiently far from the MT ends, the magnitude of the intrinsic electric field can be approximated simply as $E\simeq Q(4\pi\epsilon_0 r^2)^{-1}$, where Q represents the effective charge on the ends of a MT and r is the distance between the selected point and the end of the MT. We take, as an example, a moderately long MT consisting of approximately 10^2 dimers with a length $L\simeq 10^{-6}$ m. The effective charge Q is estimated as $Q\simeq 1.5\times 10^{-16}$ C, so that the intrinsic field is of the order of magnitude $E\simeq 10^7$ V/m. Taking into account the dielectric effects of surrounding water molecules, this value can be easily reduced to approximately $E\simeq 10^6$ V/m.

As far as the potential coefficients A and B are concerned, no reliable experimental data exist, so a rather crude estimate is made using some typical values for crystalline ferroelectrics, knowing that they do not vary substantially between different compounds. At values close to room temperature we could adopt

$$A\simeq 200\ \text{J m}^{-2},\quad B=10^{24}\ \text{J m}^{-4}. \tag{2.13}$$

On this basis we find

$$\sigma\simeq(5\times 10^{-8})E. \tag{2.14}$$

It is therefore clear that even for very strong electric fields the condition $\sigma\ll 1$ is fulfilled. The main consequence of the relative smallness of the electric field is that the propagation velocity (2.11) can be safely approximated as linearly proportional to E,

$$v=\frac{3v_0}{\gamma|A|}\left(\frac{MB}{2}\right)^{1/2}qE, \tag{2.15}$$

and is generally much smaller than the sound velocity ($v\ll v_0$). Equation (2.15) represents the Ohm-like law of linear response of kink velocity to the existing field. The coefficient of proportionality in this relationship represents the kink mobility μ,

$$\mu=\frac{3v_0}{\gamma|A|}\left(\frac{MB}{2}\right)^{1/2}q. \tag{2.16}$$

Using some representative data, we obtain

$$\gamma\simeq 5.6\times 10^{-11}\ \text{kgs}^{-1}(T=300\ \text{K}),\quad v_0\simeq 4\times 10^2\ \text{m/s}$$

$$M\simeq 10^{-22}\ \text{kg}\quad\text{and}\quad q\simeq 6\times 10^{-18}\ \text{C},$$

and hence Eq. (2.16) yields

$$\mu\simeq 2\times 10^{-5}\ \text{m}^2\,\text{V}^{-1}\,\text{s}^{-1}. \tag{2.17}$$

Thus taking $E\simeq 10^6$ V/m as a typical average value of the electric field, the propagation velocity of a kink is expected to be of the order of

$$\bar{v}\simeq 20\ \text{m/s}. \tag{2.18}$$

On the other hand, for very strong fields of about 10^7 V/m associated with the nerve axon potential, for example, the terminal velocity reaches

$$\bar{v}\simeq 200\ \text{m/s}. \tag{2.19}$$

Assuming a smooth journey from one end of a MT to the other, the average time of propagation for a single kink should therefore be

$$\bar{\tau}=L/\bar{v}\simeq 5\times 10^{-8}\ \text{s}. \tag{2.20}$$

However, increasing the length of the MT will increase $\bar{\tau}$ on two accounts: (a) increasing the numerator in Eq. (2.19), and (b) affecting the mean velocity through the dependence of the electric field on L. Indeed E is proportional to $\sim L^{-2}$, and hence v is proportional to $\sim L^{-2}$. Consequently, $\bar{\tau}$ scales with $\sim L^{+3}$, leading to a rapid increase of $\bar{\tau}$ with L.

Stability analysis of the above system shows that the discreteness of the lattice can indeed be of great importance. For example, there may exist a threshold value of the field E required to sustain kink motion. Moreover, it appears that fast-approaching kinks are more stable than slow ones. We infer that the shorter MT's have a clear advantage in the formation and propagation of kink excitations. Furthermore, by adding an external electric field parallel to a MT, one can introduce a new control mechanism in the MT dynamics. In the remainder of this paper we use an approximation of Eq. (2.9) in the form

$$u(\xi)=u_0\left[1-\frac{2}{1+\exp(\sqrt{2}\xi)}\right], \tag{2.21}$$

which is applicable to low electric fields. This expression will be of crucial importance in the analysis of the Mössbauer effect in MT's.

III. MÖSSBAUER TRANSITION PROBABILITY

Let us suppose that it is technically possible to implant a γ-active isotope (for example of Fe^{57}) into one of the MT dimers. The energy of a single γ quantum $\hbar\omega$ typically ranges from about 10 keV to approximately 5 MeV, which corresponds to wavelengths from about 1 Å to about 10^{-3} Å, respectively. It has been shown [11] that in the case of pure phonon vibrations of the chain, the Mössbauer effect is significant provided the condition $E_R<k_BT_D$ is satisfied, while in the opposite case it becomes negligible. Here E_R represents the recoil energy of the emitting nucleus, while T_D denotes the Debye temperature of the corresponding elastic lattice and k_B is Boltzmann's constant. Since the recoil energy is given by

$$E_R=\frac{(\hbar\omega)^2}{2M_nc^2}, \tag{3.1}$$

where c represents the speed of light, while M_n is the mass of a γ-active nucleus, it is clear that to have a significant Mössbauer effect the recoil energy E_R of the nucleus must be small, i.e., the γ ray should have low energy, the Debye temperature should be large, and the temperature of the experiment should be as low as possible.

The probability of the Mössbauer effect can also be enhanced by a broadening of γ spectral lines, which causes a partial overlap between emission and absorption lines. Keeping in mind that the Doppler line width ΔE_D is defined by $\Delta E_D = 2\hbar\omega(v/c)$, where v is the velocity of an emitting atom, it is clear that this effect takes place for γ rays with higher energies and for greater velocities v of emitting nuclei. We recall here that the typical spectral line width of gamma rays is $\Gamma \simeq 10^{-3}$ eV.

The aim of our investigation is to see whether the Mössbauer effect can be observed in MT's populated both by phonons and by kinklike excitations caused by GTP hydrolysis. We now set out to calculate the Mössbauer emission probability of a γ ray from the nucleus located at the dimer labelled n_0. First, we introduce the operator defining the interaction between the nucleus and the emitted γ ray in the usual way [11],

$$U_{\rm int} = \hat{G}(x_j, l_j, \hat{\sigma}_j)\exp\left(\frac{i}{\hbar}\,\vec{p}\cdot\vec{r}_{n_0}\right), \tag{3.2}$$

where the operator $\hat{G}$ depends on the position x_j, momentum l_j, and spin $\tilde{\sigma}_j$ of the γ-active nucleus labelled by the subscript j which are typical nuclear degrees of freedom. This part of the operator may be dropped from further consideration as being pertinent to the structural details of the emission process. The exponent in Eq. (3.2) contains the momentum of the emitted γ-ray $\vec{p}$ and the position $\vec{r}_{n_0}$ of the nucleus j in the dimer n_0 after the act of emission. This new position is displaced with respect to its equilibrium value $n_0\vec{R}_0$, so that

$$\vec{r}_{n_0} = n_0\vec{R}_0 + \vec{u}_{n_0}, \tag{3.3}$$

where u_{n_0} denotes the magnitude of the associated displacement. It is now quite clear that $\vec{u}_n$ determines the recoil energy released, which is related to the Doppler effect with respect to the emitting nucleus. This, thus, should essentially determine the probability of the Mössbauer resonance.

The expression for the Mössbauer transition amplitude can be calculated by the matrix element

$$M_{i,f} = \langle\psi_f|\exp\left(\frac{i}{\hbar}\,\vec{p}\cdot\vec{r}_{n_0}\right)|\psi_i\rangle, \tag{3.4}$$

where the wave functions $|\psi_i\rangle$ and $|\psi_f\rangle$ correspond to the initial and final states of the nucleus, respectively. These functions represent eigenstates of the chain dynamics which strongly depend on the dimer's displacements in the neighborhood of the emitting nucleus. A Mössbauer transition occurs when a $|\psi\rangle$ state remains unchanged before ($|\psi_i\rangle$ and after $|\psi_f\rangle$) the emission, so that the γ-ray involved absorbs the entire energy of transition. In other words, the emission is an elastic process. The wave function may be represented as a tensor product of the function (2.21) and describing kinklike excitations in MT and the quantum phonon states, i.e.,

$$|\psi\rangle = |\varphi\rangle\prod_q |v_q\rangle, \tag{3.5}$$

where $|\varphi\rangle$ is determined in terms of function (2.21) and

$$|v_q\rangle = \frac{(b_q)^{v_q}}{(v_q!)^{1/2}}|0\rangle, \quad v_q = 1,2... \tag{3.6}$$

with b_q and b_q^+ representing the annihilation and creation operators, respectively, for longitudinal phonons with a wave vector q. As usual, $|0\rangle$ denotes the phonon vacuum. Consequently, the net displacement $\vec{u}_{n_0}$ can be seen as composed of two contributions, classical and quantum, as follows

$$\vec{u}_{n_0} = \vec{u}_{\rm cl} + \vec{u}_{\rm qu}, \tag{3.7}$$

where $\vec{u}_{\rm cl}$ is defined by kinklike excitation, while the quantum component $\vec{u}_{\rm qu}$ is due to phonons and takes the standard form

$$\vec{u}_{\rm qu} = \sum_q \left(\frac{\hbar}{2MN\Omega_q}\right)^{1/2}(b_q + b_{-q}^+)\exp(iqR_0n_0). \tag{3.8}$$

This approach makes sense only if we assume that the entire dimer including the emitting atom moves as whole. In this case M denotes the mass of the dimer, and N the number of dimers in one protofilament while the acoustic phonon dispersion relation is taken in the usual linear form $\Omega_q = v_0|q|$.

In this case, from Eq. (3.1) it follows that E_R has a very small value, since $m_N \sim M \sim 10^{-22}$ kg. If the γ-ray energy (e.g., for Fe^{57} it is 14.4 keV), this would mean that $E_R \sim 10^{-26}$ J, which is much smaller than k_BT for room temperatures.

However, in reality the emitting atom is not necessarily tightly bound to the rest of the dimer, so that the above estimate has indeed been overly pessimistic. Nevertheless the contribution of phonon's degrees of freedom can be represented by

$$\langle M_{\rm qu}\rangle = \exp(-\beta Q^2\cos^2\theta), \tag{3.9}$$

where β represents a complicated Debye-Waller factor, $Q = p\hbar^{-1}$, and θ is the relative angle between the displacement $\vec{u}_{qn}$ and the γ ray's momentum $\vec{p}$.

The Debye-Waller factor has a simple enough form only in the idealized case of rigid dimers, where

$$\beta = \frac{1}{4}\sum_q \left(\frac{\hbar}{MN\Omega_q}\right)\coth\left(\frac{\hbar\Omega_q}{2k_BT}\right). \tag{3.10}$$

Otherwise, this factor must be much greater, since M has the order of magnitude in the range 10^{-25}–10^{-27} kg depending on the structural details of the tubulin protein comprising each dimer. In this case the frequencies Ω_q may be higher due to smaller masses of the atoms involved.

Now, we wish to examine the contribution of the classical kink dynamics to the effect. First we determine the function φ_n as a relative displacement of the neighboring dimers

$$\varphi_n=\frac{u_{n-1}-u_n}{R_0}=\frac{\partial}{\partial x}\,u(x,t), \tag{3.11}$$

or, using the dimensionless variable ξ,

$$\varphi(\xi)=-\frac{\partial}{\partial\xi}\,u(\xi)\,\frac{\partial\xi}{\partial x}, \tag{3.12}$$

where $u(\xi)$ is represented by Eq. (2.21). After simple calculation one obtains

$$\varphi(\xi)=-2\sqrt{2}\,\alpha u_0\,\frac{\exp(\sqrt{2}\xi)}{[1+\exp(\sqrt{2}\xi)]^2}, \tag{3.13}$$

so that the classical contribution can be written as

$$\langle M_{\rm cl}\rangle=\langle\varphi(\xi)|\exp\left\{i\,\frac{p}{\hbar}\,u_{\rm cl}\cos\,\theta\right\}|\varphi(\xi)\rangle. \tag{3.14}$$

Performing the requisite calculation yields

$$\langle M_{\rm cl}\rangle=\frac{4}{3\sqrt{2}}\,u_0^2\alpha^2\left[1-\frac{1}{10}\left(\frac{p}{\hbar}\right)^2u_0^2\cos^2\theta+\frac{1}{280}\left(\frac{p}{\hbar}\right)^4u_0^4\cos^4\theta\right]. \tag{3.15}$$

Hence the total matrix element is now obtained, using Eqs. (3.9) and (3.15), as

$$M_{i,f}=\frac{4}{3\sqrt{2}}\,u_0^2\alpha^2\left[1-\frac{1}{10}\left(\frac{p}{\hbar}\right)^2u_0^2\cos^2\theta+\frac{1}{280}\left(\frac{p}{\hbar}\right)^4u_0^4\cos^4\theta\right]\exp\left[-\beta\left(\frac{p}{\hbar}\right)^2\cos^2\theta\right]. \tag{3.16}$$

Since the probability of a Mössbauer transition is given by

$$W_{i,f}=|M_{\rm cl}|^2|M_{\rm qu}|^2, \tag{3.17}$$

the final step in our calculation of the Mössbauer transition is to perform averaging with respect to all angles ϕ and θ corresponding to a random distribution of propagation directions of the emitted γ radiation. Therefore,

$$\overline{W}_{i,f}=\int\,\frac{d\Omega}{4\pi}\,W_{i,f},\quad d\Omega=\sin\,\theta\,d\theta\,d\psi. \tag{3.18}$$

Through the substitution $z=\cos\,\theta$ the calculation reduces to just three types of integrals as follows:

$$I_1=\int_{-1}^{+1}dz\,\exp(-Dz^2),$$
$$I_2=\int_{-1}^{+1}dz\,z^2\exp(-Dz^2)=-\frac{\partial}{\partial D}\,I_1 \tag{3.19}$$

and

$$I_3=\int_{-1}^{+1}dz\,z^4\exp(-Dz^2)=-\frac{\partial^2}{\partial D^2}\,I_1, \tag{3.20}$$

where we introduced the dimensionless Debye-Waller factor $D=\beta(p/\hbar)^2$. Using the error function $\phi(\lambda)=(2/\sqrt{\pi})\int_0^\lambda\exp(-t^2)dt$ results in the expression

$$\overline{W}_{i,f}=\frac{4}{3\sqrt{2}}\,u_0^2\alpha^2\left\{\frac{1}{2}\left(\frac{\pi}{D}\right)^{1/2}\phi(\sqrt{D})+\frac{1}{10}\,\epsilon^2\,\frac{\partial}{\partial D}\left[\left(\frac{\pi}{D}\right)^{1/2}\phi(\sqrt{D})\right]+\frac{1}{10}\,\epsilon^4\,\frac{\partial^2}{\partial D^2}\left[\left(\frac{\pi}{D}\right)^{1/2}\varphi(\sqrt{D})\right]\right\}, \tag{3.21}$$

where we introduced

$$\epsilon=u_0\,\frac{p}{\hbar}. \tag{3.22}$$

IV. DISCUSSION AND CONCLUSION

This nonlinear model was first introduced [8] in order to try to explain some of unambiguously nonlinear features of MT dynamics. On the basis of that model some interesting biophysical phenomena regarding living cells were explained [14–17].

We assumed in the present paper that γ-active nuclei capable of emitting soft γ rays can be embedded in dimers of MT's. The main objective of our study has been to evaluate the probability of the Mössbauer effect for such a system, provided that both the phonon modes and kinklike excitations exist in it.

First of all, we can discuss the broadening of the spectral lines by the Doppler effect caused by the motion of the emitting atom together with a dimer due to the propagation of kinklike excitations. We can estimate the average velocity of dimers involved in kink excitation on the basis of Eq. (2.21) for dimer displacement. After a simple calculation we obtain

$$v_D\sim u_0\alpha\overline{v}. \tag{4.1}$$

Taking $\overline{v}\simeq 20$ m/s, $u_0\simeq 5\times10^{-11}$, and $\alpha\simeq 0.5\times10^{10}\ \mathrm{m}^{-1}$, one finds

$$v_D\simeq 6\ \ \mathrm{m/s} \tag{4.2}$$

For extremely high values of the velocity (2.19) we expect $v_D\simeq 60$ m/s. Thus the broadening of the line is expected to be $\Delta E_D=2(\overline{v}/c)\hbar\omega\simeq10^{-3}$ eV for $\hbar\omega=10$ keV, and $c=3\times10^8$ m/s or even 10^{-2} eV for the axon action potential field. If we compare this with a typical natural width of a spectral line $\Gamma\simeq10^{-3}$ eV, we see that Doppler's broadening should cause additional overlap between emission and absorption lines, giving rise to Mössbauer transitions. We now discuss the consequences of Eq. (3.20).

The factor $(3/3\sqrt{2})u_0^2\alpha^2$ is approximately 0.1, and its origin is due to kink motion, since u_0 and α are obtained using the kink's parameters. The decisive factor in the determina-

tion of the magnitude of the Mössbauer transition is thus the Debye-Waller factor D. If we analyze the phonon dynamics of dimers we can bear in mind that each dimer is a globular protein with a molecular weight of about 110 kD; hence each dimer should possess a large set of vibrational degrees of freedom. Some of them may result in global phonon modes through the entire MT, while others can remain local [18]. Global (phonon) and local (vibron) excitations can be converted into each other due to nonlinearity inherent in the MT structure. The periodic structure of MT's should thus result in a definite spectrum of global phonon mode maxima. Samsonovich, Scott, and Hameroff [19] reduced the phonon dynamics of a MT to the very simple global phonon spectra whose eigenvectors are standing waves of the simplest form:

$$\varphi_n=\left(\frac{2}{L}\right)^{1/2}\sin\left(\frac{\pi n x}{L}\right), \quad n=1,2,..., \tag{4.3}$$

where L is the length of a MT. If we accept that such an approximation holds, we can estimate D for $\hbar\omega=10$ keV as a function of temperature. Since we estimate

$$\left(\frac{p}{\hbar}\right)^2=2.5\times10^{21}\ \ \mathrm{m}^{-2}, \tag{4.4}$$

β can be estimated as follows:

$$\beta\simeq10^{-23}\ \ \mathrm{T(m^2)}. \tag{4.5}$$

Thus we have

$$D\simeq2.5\times10^{-2}\ \ \mathrm{T}. \tag{4.6}$$

On the other hand, ϵ is estimated to be

$$\epsilon\simeq\tfrac{1}{2}. \tag{4.7}$$

So we finally have

$$\overline{W}_{i,f}=0.1\left\{\frac{1}{2}\left(\frac{\pi}{D}\right)^{1/2}\phi(\sqrt{D})+\frac{1}{40}\frac{\partial}{\partial D}\left[\left(\frac{\pi}{D}\right)^{1/2}\phi(\sqrt{D})\right]\right\}. \tag{4.8}$$

At room temperature ($T=300$ °K), $D\simeq7.5$, and one obtains

$$\overline{W}_{i,f}=0.1\left\{\frac{1}{2}\left(\frac{\pi}{7.5}\right)^{1/2}\phi(\sqrt{7.5})+\frac{1}{40}\frac{\partial}{\partial D}\left[\left(\frac{\pi}{D}\right)^{1/2}\phi(\sqrt{D})\right]_{D=7.5}\right\}. \tag{4.9}$$

Since the error function could be fairly well approximated by unity, the final expression (4.9) yields the numerical estimate

$$\overline{W}_{i,f}\simeq3.2\times10^{-2}, \tag{4.10}$$

which indicates that under the conditions where high enough population of kinks exists, the Mössbauer transitions would be detectable. If the intrinsic electric field takes extremely high values on the order of 10^7 V/m, the kink velocity would approach the sound velocity remarkably, increasing the parameter α and consequently the probability of Mössbauer transitions. For example, in the case of the nerve membrane the resting membrane potential difference is 0.1 V (the membrane is 75 Å thick) which implies a strong transmembrane electric field of about 10^7 N/m. In this case we estimate that

$$\overline{W}_{i,f}\simeq0.1 \tag{4.11}$$

leading to the encouraging conclusion about the feasibility of a successful Mössbauer effect experiment stated above [20].

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