Molecular Motors and Quantum Mechanics

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Introduction

Molecular motors - myosin, dynein, and kinesin - have been studied with regard to the mechanism by which the motors are powered. In muscles, the myosin molecule provides the power of contraction, while in dynein and kinesin the power transports cargo within the cell along microtubule filaments. The following is limited to kinesin, but is applicable to both myosin and dynein.

The kinesin molecule has twin heads and moves towards microtubule plus end using a hand-over-hand walking action that can do work [1,2]against loads of up to 7 pN. In the manner of Brownian motion, the motor is thought to diffuse back and forth on a spring-like tether using thermal energy from the bath to stretch out the tether, locking on to the track as the spring is stretched out, and then the motor advances while maintaining its grip on the microtubule as the spring relaxes. In the alternative, a change in the neck linker molecular conformation is thought to convert Brownian motion to advance the motor.

The free energy of docking the neck linker to the microtubule is found [3] very small while MD simulations [4] show forces in unbinding are very large and consistent with clamp experiments. However, MD simulations of the conversion of thermal energy into motor motion do not show how ATP hydrolysis produces the energy for the power stroke that comes from thermal fluctuations. Instead, thermal energy is simply assumed to control the force developed from Brownian motion while thermal vibrations allow searching for a binding site, and during or after completion of the power stroke, thermal fluctuations dislodge the kinesin from the microtubule. But how this occurs is not found anywhere in the literature.

Currently, the general belief is that Brownian motion induced by thermal fluctuations is important in the motion of kinesan motors. However, electrostatic forces from chemical additives to the bath can induce charge to steer [5] the neck linker and coiled tether to the microtubule are also important. Indeed, additives that make the neck linker and tether more positive were found to increase motor motion while negative charge decreased the motion. However, some kinesins [6] have neutral coiled tethers, yet still show increased motion suggesting that another region of the molecule may perform this tethering role. But explanations of how electrostatics affects motor motion is not well understood.

Proposal

Simple QED induced EM radiation [7] produced in nanoscale structures is proposed to explain molecular motors. Simple QED is a consequence of the Planck law of QM that requires the nanoscale neck linker and coiled tether to charge positively directly from ATP binding or even from heat in the water bath. QM stands for quantum mechanics. The QM charging of the neck linker and coiled tether occurs even if chemical additives are not included in the bath as would be the case for neutral coiled tethers. Indeed, charge is induced in all nanoscale structures because QM requires the heat capacity of atoms in the nanostructure to vanish thereby precluding any conservation of absorbed heat by an increase in temperature. Simple QED stands for quantum electrodynamics of real photons differing by simplicity from Feynman's virtual photons. Simple QED conserves heat from ATP hydrolysis or thermal heat of the bath by creating EM waves that by the minimum time principle of Fermat stand across the minimum dimension of the nanostructure, e.g., across the diameter of neck linker and coiled tether.

Basic motor electrostatics is illustrated in Figure 1. Since the simple QED radiation exceeds the respective ionization potentials, electron loss charges the coil and linker positive, and since the

microtubule carries a negative charge, electrostatic attraction pulls the tether downward to the microtubule. Upon contact, the neck linker acquires the negative charge of the microtubule and is repelled then allowing the neck linker to acquire a positive charge for the next microtubule contact.

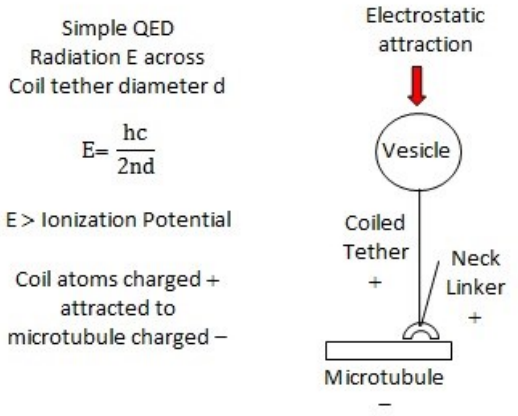

Figure 1 Simple QED charging of coiled tether

An enlarged view of electrostatic molecular motor mechanism is illustrated in Figure 2. The neck linker comprising Head 1 and Head 2 is shown in gray moving in the forward direction along a microtubule of α+ and β- tubulin dimers. The coiled tether shown as a black line connects the neck linker to the vesicle carrying the cargo. Head 1 on the left is shown charged negative and bound to the first β- tubulin site, but because of subsequent mutual repulsion Head 1 is shown moving upward. Head 2 and the coiled tether are charged positive by simple QED with Head 2 attracted to bind a the second β- tubulin binding site. At this time, Head 1 in a hand-over-hand motion moves toward the third β- tubulin binding site. Since both α+ and β- tubulin dimers are about 8 nm in length, Head 1 moves over 2 of the α+ tubulin sites or 16 nm in the forward direction.

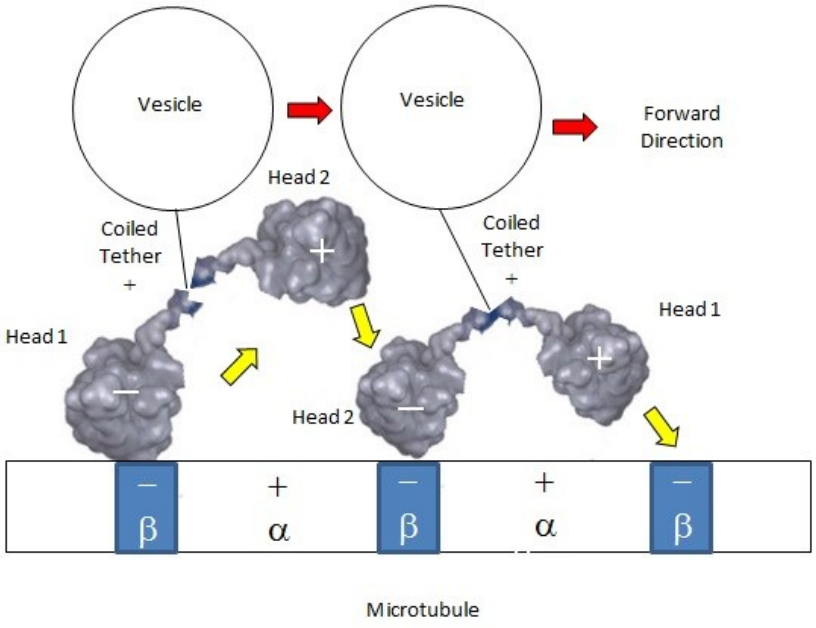

Figure 2 Molecular motor electrostatic mechanism

Discussion

Simple QED based on the vanishing heat capacity of QM at the nanoscale offers a rational basis for understanding the motion of molecular motors is electrostatic. Although electrostatics is proposed [1,5-6] to explain the motion of molecular motors, simple QED unequivocally shows the underlying physics is electrostatics finding basis in the QM fact the heat capacity of atoms in the nanostructures vanishes at the nanoscale. The literature is replete with molecular motion being caused by random Brownian motion consistent with classical physics, but nanoscale motors follow QM.

Simple QED shows heat from the thermal bath cannot be conserved in kinesin heads and the coiled tether by an increase in temperature, the consequence of which is conservation proceeds by creating standing EM radiation inside and across the minimum dimension of the nanostructure based on the Fermat principle that conservation of energy proceeds in the shortest possible time. For the coiled tether, the EM radiation E is confined across the tether diameter d while in the spherical heads is confined across their diameter d, i.e., $E = hc/2nd$, where h is Planck's constant, c the speed of light, and n the refractive index of the nanostructure. Since $d < 100$ nm, the Planck energy E is beyond the UV and ionizes the nanostructure atoms, the loss of electrons producing positive charge.

Heat Q supplied to molecular motors is generally thought caused by ATP binding to their surfaces. But heat Q from the thermal bath activates simple QED charging even though QM precludes an increase in temperature as conservation of energy requires the heat to be conserved by another form of energy, as in the instant case of molecular motors the form is EM radiation E. The thermal heat Q corresponds to raising the temperature of each atom in the nanostructure to bath temperature T in Kelvin. For Na atoms, $Q = 1.5$ kT Na, where k is Boltzmann's constant. Hence, the number Np of simple QED photons is, $Np = Q/E$ charges the nanostructure by the photoelectric effect.

Based on free energy, the neck linker docking onto the microtubule is thought [3] to be small because the large, favorable enthalpy changes ΔH are balanced out by large unfavorable entropy ΔS changes . Enthalpies were calculated by creating Van't Hoff plots of R ln K versus 1/T where K is the ratio of mobility to immobility. Entropies were calculated using $\Delta G = \Delta H - T\Delta S$. However, the enthalpies are questionable as temperatures are precluded by QM. Modification of Van't Hoff methodology for charge induced attraction in binding and repulsion in unbinding is required.

MD simulations have long claimed to provide explanations of atomic interactions. However, this has always been questioned as classical physics and not QM is used in MD simulations of heat transfer at the nanoscale. Notwithstanding the fact the mechanism by which ATP binding, hydrolysis, and product release are converted into mechanical force is not known, MD simulations based on classical physics claim [4] with certainty large pulling forces $>$ 440 pN are required for unbinding. Contrarily, QM induced charge repulsion should have been included for protein unfolding of molecular motors.

References

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