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Chemical and Molecular Physics in Perspective Quantum Mechanics is alternative of Quantum Classical Mechanics

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Abstract

The concept of quantum transition is based on the completion of a succession of time dependent (TD) perturbation theories in QM. This sequence coheres in atomic and nuclear mechanics because quantum transfers have no dynamic by nature. The kinetics of "quantum" transition, which are dictated by the coupled motions of a lightweight electrons and very massive nuclei, are inherent by nature in chemical and molecular physics, and the sequence of TD perturbation theory become unique. The dynamics problem for reference frames in the QM approach is an exception, because the electronic subsystems is "removed" from the main dynamic system and hence is not physically filled: it just produces an electromotive force wherein the nuclei oscillation. There are two approaches to get rid of the abovementioned singularities. The first way involved adding an additional assumption into molecule quantum theory in the shape of the Franck-Condon rule, which use the isothermal approach. The author developed the second strategy, which involved injecting chaos to dampen the unique dynamically of the bonding movement of electrons and nuclei in the intermediary state of molecules "quantum" transition. Dozy pandemonium is a type of chaos that occurs solely during molecular quantum events. Technically, damping is accomplished by substituting a finite quantity for an endlessly small imagined additive in the spectrum form of the state's full Green's functional. In the molecule transient stage, damping chaos leads to energy spectrum consistency, which is an indication of classical physics. However, in the adiabatic approach, the molecule's starting and end states follow quantum physics. Quantum-classical mechanics is a branch of molecule quantum theory that consider dynamics of the transitory molecular states of "quantum" transition. Dozychaos technicians of primary education electron carriers in crystalline materials, which is the easiest case of DC (dozy-chaos) mechanical systems, and its implementations to a broad variety of cases, including the absorption spectrum in dyes of polymethine and their collection, have previously demonstrated the effectiveness of the dampers for the above said beginning of the universe. This study explains the elementary electron DC mechanics exchanges in a systematic way. The key results of its implementations are also discussed, as they were in the introductory.

Keywords

Quantum Physics; Singularity; Dozy Choas; Electron Transfer; Molecular Physics.

A novel theoretical framework for molecular quantum shifts and its applications has been developed. Quantum theory is one of the most significant fields of current theoretical physics, but not the most important. Atomic science, nuclear physics, and material science known as quantum mechanics provide a crucial foundation for recent and current technological advancements in the twentieth century. As a result, in a wide scientific context, quantum mechanics' potential are thought to be nearly endless. QM can be applied to

anything, including the entire cosmos [1-4] as well as the human mind and mind [5-9]. In scientific discovery, the term "quantum" is widely popular [4]. In essence, there is a widespread belief in the science establishment that QM provides the final and definitive word on the nature of reality [9]. The current research examines the limitations of quantum mechanics' application by examining the intrinsic conflicts that appear when it is used impartial to a variety of molecular and chemistry physics issues. The issue is just sketched out in the beginning. A full explanation both on qualitative and quantitative levels will be included in the following parts. The primary application findings for the new approach offered by the writer in theory are shown in this part. This approach contrasts from the standardized way, in which the theory is provided first, followed by examples of its applicability to the study. Because the majority of new findings have already been published [10-19] and presented at international meetings [20-36], this is the case. This story is based on articles and reports showing the new current theories performance in experiments, and it aims to explore the new challenge in physics at a higher physiological level, as well as provide a prominently explanation of the theoretical in basic electron carriers in crystalline materials. There are 2-key reasons why this case should be simplified [11,18]. In the instance of a free electron, the first entails estimating the atom's Green's functional by it. The second is concerned with only evaluating nuclei's quasi vibrations while ignoring their local oscillations. As according molecule and molecular physics, a novel theoretical technique to studying molecule quantum shifts and basic electron transfer in crystalline materials has been developed. This novel method to concept is known as dozy-chaos physics, or quantum classical technicians. The enforced integration of quantum-classical mechanics into molecule and chemistry physics is linked to the removal of a crucial discontinuity in the probability per unit time in the coefficients of quantum transition in molecules. The exceptional of the energies of nuclei and electron, as well as their simultaneous motions the processes of quantum particles jumps, gives birth to this anomaly in quantum theory when it goes further than the adiabatic approach. The paradox is removed by replacing the infinite imagined addition I with its infinite quantity in the spectrum of the entire molecule Green's function [10-12]. When the scientific idea is compared to tests, it is discovered that the modulus of this imagined additive is substantially larger than that of the quantum of nuclear fluctuations: >> [14, 28, 34]. The quantity of could be interpreted as the energetic width of the transitory state's particle virtual levels, which allows for various exchanges of movement and energy among distinct nuclei and electron vibrational modes. However, due to the previously indicated extremely large quantity of, this transfer of movement and energy crashes, creating mayhem in the movement of both nucleus and the electron undergoing the transition. Dozychaos is named by the fact that it is missing in the beginning and end states and only appears in the midst of quantum particles transformations [14, 28,33]. In synthetic thermodynamics, the writer demonstrated the effectiveness of the damping technique for the above said beginning of the universe using an instance of the scientific revelation of primary school electron carriers in crystalline materials and its application [10-19,28, 29, 34, 35] to the spectra in poly-methine colourings and their aggregates [37-44], as well as its application forms [20, 34,45] to a variety of many other basics result [46,47]. The above quantum changes in quantum physics are, speaking literally, quantum-classical transition process, since, while their final and initial nations are quantum, their temporary states are conventional. The quantum essence of the original and final nations is evidenced in the reality that these nations are commonly discussed by QM in the adiabatic estimate, and the framework of the final position of the molecules varies noticeably from the framework of its preliminary state of the reorganisation of the nuclear sub-system. Chemical changes that result in the production of small compounds are a good example of such. The chaos existence in the movement of electron implicated in the QC (quantum Classical) transformation is affiliated with the traditional nature of the transient condition of molecules, which did lead to a spectrum ranging of their energy sources in this transient condition [16, 18, 36, 48, 49]. QC mechanics, also known as gormless mechanics, is the concept that explains subatomic transitions. The basic issue in quantum-classical mechanics is the dozy-chaos concept of basic electrons carrier in crystalline materials, which will be discussed in depth in the following sections. QC mechanics reveals a slew of basic experimental facts in chemistry that previously

eluded understanding within the boundaries of ordinary quantum theory of electron-nuclear movement. Experimental results on the form of the optical pop acts of polymethine (PM) colourings and their granules in remedies can be explained using quantum-classical fundamentals, wherein the quantum-classical shifts in their structural and optical properties fluorophore(FP) can be estimated by primary school particle procedures in crystalline materials [10-15,18,28]. Exciton effects appearing in many situations as a consequence of molecule agglomeration complicated but do not drastically change the overall view of basic quantum-classical transition in dye FP [10-15,18,28]. Dahne [50] proposed the notion of an ideal polymethine nation to models the electrical properties of the basics optical FP in PM colourings, their PM joint, whereby there is an obviously elongated allocation of the concentration of the -electron control all along quasi-linear polymethine sequence. After optical stimulation, this density varies frequently along the link and is reallocated alternatively [51]. Furthermore, the electronic shift for the initial excited state is concentrated on the chains [51]. As a outputs, the electrical transitions to the initial excited state can be approximated by the fundamental transfer of electrons along the chain [10-15,18,28]. The polymethine colors that will be explored here can be thought of as Dahne's optimal polymethine condition. Because the total transmission of interchanging charge along full chain in a perfect PM state comprised of acts of primary school charge transport over a short distance among two carbon particles, the tunnelling effects in an electrons transfers are slight, and Gamow's tunnel component is close to the expected value [10-15,18,28]. Because of the stationarity and adequate path of the basic optical FP of PM dyes and agglomerates, as well as the stationary and adequate distance of their polymethine chains, we can ignore the interplay of the electron transitions with the movement of the dyes' atoms and only consider its interplay with enviro nuclei [10-15,18, 28]. The most significant outcomes are conceptual optical spectroscopy on PM dye monomer units [12,14,15,18,28,41-43] (Figs.1. and Fig.2.), dimmers[15,29,42,43], H+ tabulates (Fig.2.)[16, 18, 29, 42, 43], and J agglomerates (Fig. 2) [10-12, 14, 17, 18, 28, 29, 37-40, 42, 43], as well as theoretical spectra. The essence of the well-established limited J-band (sFig.2.) is ascertained by the vibrant pumps of electron transitions in the fluorophore of J aggregate particles with mildly chaotic highly organised movement of nuclei in the surroundings [10-12, 14, 18, 28]. Exciton effects play a minor influence in the formation of the J band. The presence of dozy-chaos dynamic as well as a decent sized exciton dynamic, as well as their significant interference interactions [16, 18, 29], elucidates the structure of the restricted H*band (Fig.2.). In the FP of the H*accumulation, which is the dimer, a competitor intervention of the chaotic kinetics of nuclear reorganisation and exciton interplay lead to a "hydrostatic chaos" from the peaks of the electro - optic band of the H* dimmers into its airfoil, trying to make the high point even slimmer and the wing even broader. The exceptionally excitons connection in the H* dimmers, which is a result of the unique structures of the H*monomer that make this up, is linked to this phenomenon. The H*monomer are cyclic biphenyl with a very wide optical fluorophore area [42]. As a output of the high exciton contact of the H*subunits in the H * dimer, the maximum of its study of optical bands narrows as a outcome of "pump pandemonium" from the top into the bands wings [16,29]. The remarkable outcomes of QC mechanics are the outcomes of trying to explain the resonance behaviour of the contour of the optical bands of the PM dye polymer as a outcome of changes in the duration of its PM sequence [12,18,41] (Fig.1). Although the soppy QM transition in the mentioned organic material appear to be quite advanced, this substance, in its dynamic nature rates in subatomic physics like a H2 ion in structure nature in QM [33b], seems to be quite simple. The interactions of QC shifts becomes weakly reliant on dozy turmoil in the presence of strong DC, and the installed of the complete electron nuclear magnitude of transformation can be equipped by the Gamow's corridor exponent, which is reliant on the transitory phonon surroundings. This simple method allows us to avoid considering the fictitious spectral additive portrayal of the full Green functions, and to express the physical study of the transitory state in terms of a large numbers of corridor and over barriers electricity states that provide the "quantum" transformation of a primary school charged particles, rather than dozy chaos. This technique [52] was devised long before the advent of QC physics [12,15,28], and we can now argue that the notion of a significant number of tunnels or over state is the most

basic version of DC. In 1990, a conceptual explanation of a basic study trends in the Bronsted equations [47] for proton transfers processe was published [45], based on this approach [52]. Bronsted and Pedersen discovered the Bronsted connections in 1924. (see Ref.[47]). Ref.[52] has a theory that is instantly applicable to the understanding of electron carriers. Because of changes in the barrier width, thermic variations of the barrier layer quality must be included to understand the reactions of heavy particle transfer. Since of changes in the barrier width, thermic variations of the barrier layer quality must be included to explain all reactions of heavy particle transfer. Because of the huge scale of the electrical wave functions in the beginning and last states, the electrons transfer is sensitive to minor fluctuations in the white and gray chain link, unlike the fundamental protonation. The notion of a significant number of tunnels or over states, as well as acoustic frequencies dispersal and barriers width changes, explain the experimentally determined significant amount of flatness of the Bronsted relations. Our theory's estimated dynamic isotope effect agrees with experimental results [45]. The regularities of base-acid interactions are sometimes connected with electron carriers rather than proton transfers [45]. Ref. [45] lays out the criteria for choosing one of several response mechanisms. The theory of acid treatment can be extended to electrochemical processes by taking into account the well-known similarities of Things in different ways and Tafel's law correlations in redox reactions [45].

Main Text:

The idea of dozy chaos and the structure of molecular atomic transition. Many physicists thought the physical image of the universe was full or almost complete just at end of the nineteenth century. Classical mechanics were used to create this physical representation of the world. Nevertheless, the theory of a completely black brain's equilibrium radiation, the issue of so ultraviolet disaster, and the stability of light velocity and its freedom from stationary reference movement remained unsolved. As a result, the theory of general relativity and quantum mechanics were born. Quantum mechanics paved the way for atomic and nuclear physicists to emerge. Quantum theory also served as the foundation for molecule physics, which grew fast in 2 ways. The first was linked to the Born-Oppenheimer isothermal assumption [53], that was used to explain the structure of the molecule and solid. The other was linked to the Franck-Condon theory in molecular spectroscopy [54,55,56,57]. The isothermal approach, wherein the movement of light protons swiftly adapts to a slow movements of nucleons and which most often accurately characterises the stable level of molecular systems, adheres to quantum mechanics' rules. According to the Franck-Condon (FCn) principle, a light electrons makes a quick quantum jump to an exciton after optical radiation of a molecules, and then the entire structure of nucleons in the molecules slowly adjusts to the different distribution of electron in the exciton. In many circumstances, this hypothesis leads to good concordance between theoretically and experimentally molecular spectra.

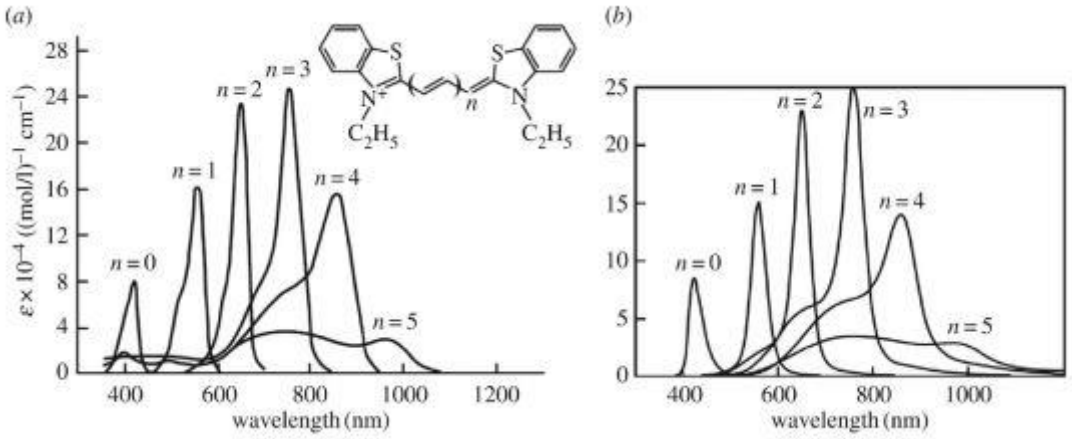

Fig.1. Qualitatively, [12,41,43] (a) quantitatively monomers optical absorptions spectrum dependent ont the length of the polythine chains.

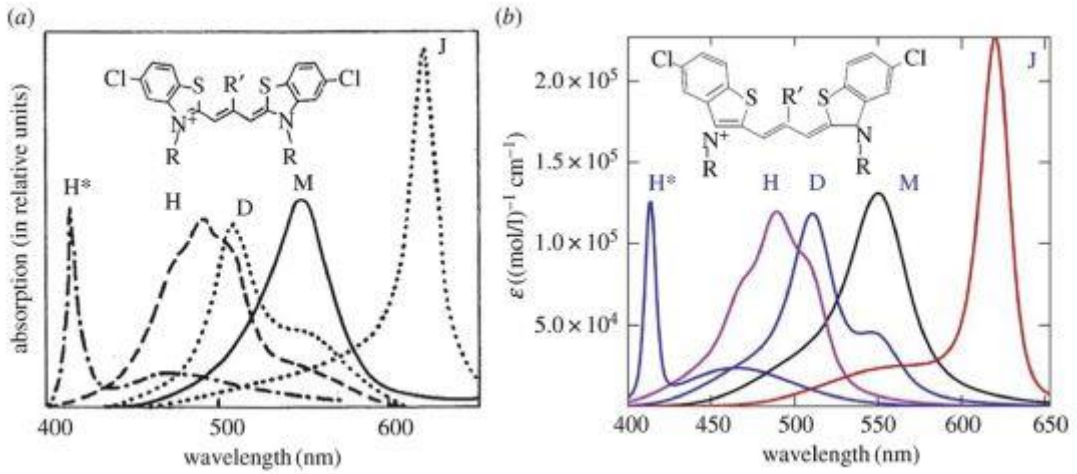

Fig.2. Optical absorptions spectrum [18,19,29,35] (b) in thiapolymethine cyanines adjusted to the fundamental information (a) on PM dye monomer.

With exception of atomic absorption spectroscopy, in which the interactions of a quantum transformation are of little importance and are already calculated by the FCn principle,2 in spectroscopies, the interactions of a quantum transformation are of great significances and are already ascertained by the FCn principle. 3 Despite the fact that the FCn kinetics of the quantum transitions raise a No. of a priori physiological objection, the theory's excellent correlation with experiments has made it a "unwavering" physical postulate inside molecular quantum theory for nearly a century. Thus, the widely accepted principle of molecule quantum transition has a long background history that can be traced back to well classical writings of Born and Oppenheimer (BO) [53] and Condon and Franck [54-57], which were published shortly after the field of QM underpinnings. BO was the 1st one to solve the subatomic problem for a systems of linked electron in the simple form for molecule [53], introducing an effectives and practical physically techniques that would later be known as adiabatic approximations. Ehrenfest [60] had already formulated isothermal symmetries, which gave rise to adiabatic approximations. The BO hypothesis of a notable differences in the general public of atomic nucleus, which allows the detachment of the slow motions of really heavy nucleus from the motions of gentle electron by ignoring the small non adiabaticity user in the Governing equations to solves subatomic troubles, explains the efficacy of heat transfer approximation. Modern solid-state mechanics and material sciences are based on the BO hypothesis [53]. With the work of Condon and Franck [54-57], the based of so FCn principles, an entirely new image emerges. The kinetics of molecular quantum transition are divided into two stages, as stated previously, due to the large disparity in electron and nuclei weights. Under the impact of an exterior perturbation, a fast electron enters an activated electronically quantum state almost instantly in first step. In the second phase, the nuclear subsystems of the molecule undergoes so-called reorganisation, wherein the spatial structure of the heavy nuclei gradually adjusts to the new conduction electrons. A picture like this, on the other hand, poses a severe objection. Because of the nuclei's considerable inertia, they would not follow the electron's movement, but will simply restore the electrons to its former condition as quickly as possible [14,28,33b]. In those other side, based on these basic arguments, the chance of a molecule quantum shift must be 0. Nevertheless, if the heavy nucleus start moving after a light electron which is already in the exciton, the nuclei's high inertia prevents them from stopping in the excited states [14, 28, 33b]. In other terms, the chance of a molecule quantum shift must be unlimited. Thus, these basic and wide quantitative considerations show that the rates of molecule quantum events have a singularity. Due to the effectiveness of the FCn theory in practically uses, which led in the developments of contemporary molecules spectroscopies, these ideas were either not addressed or not regarded at one point. Nonetheless, the applicability of the FCn rule remains an open

subject in principle. In this light, the FCn rule should be seen as an economical assumption rather than a physical rule that lacks a complete theoretical foundation. There is no explicit numerical support for the FCn principle in concept, in addition cited subjective difficulties. It is important to address the issue of the transient kinetics condition in molecule quantum transition statistically, at least in the some simplest circumstances, based on quantum mechanics' initial concepts. Furthermore, such a system, demonstrating the FranckCondon principle in particularly, should be proved across a variety of applications. To yet, though, really no solution was found. According to the subjective physical question, "Under what conditions is a light electrons capable of moving nuclei with significant inertia and therefore allowing nuclear subsystems reconfiguration in molecules quantum shifts?" [14, 28, 33b]; [14, 28, 33b]; [14, 28, 33 The electron should forsake efforts to move the nucleus "alone" in favour of inducing movement in same nuclei. How can this happen if the atoms in the molecular are vibrating at least once a second at all temperature of up to 0? During the molecule phase transition, the vibration movements of oscillating nuclei must be translated, at least to some extent, into the displacement of their equilibrium places in order to alter their equilibrium locations in spacetime. If indeed the nuclei's motions are erratic during in the molecular quantum shift, this is simple to implementation. When the nuclei's oscillations are disorderly, an electron can readily regulate their movement during "quantum" phase. Electron that connect nucleus to molecules produce erratic motion in nucleus in a transitory state, as indicated by the theoretical model, which will be described later. In other terms, throughout a molecular "quantum" shift, a light electron organises the motion of highly heavy nuclei by creating chaos, culminating in this change. This is the basis of molecules quantum events' identity. This happens when an electrons in a brief molecular state causes confusion. This is referred to as dozy pandemonium. In the transitory state of molecules undergoing quantum jumps, dozy pandemonium is the combined effect of the aggregate chaotic mobility of atomic nuclei, as well as their chaotic EM interactions. Since electrons and nucleus are ubiquitous, dozy chaotic is a global physical event [14-18,28,32-36,48,49]. There are some a priori objections to the originally provided subjective logic, which leads to the conclusion that molecular transition probabilities are unique. This objection asserts that, despite their significant rigidity, nuclei cannot come back an enthused light electron to its initial surface state because the particle has already entered the well quantum system in which it can flee attributed to the prevalence of a bandgap energy in the electron density, as described by QM. As a result, the electron inside the exciton is required to gradually adjust the nuclear systems towards its new charge density. This is what the FCn concept is all about. Our a priorioty criticism, as well as the Franck-Condon rule itself, are predicated completely on the a prioriorty premise that QM is valid in this circumstance. As stated past, there is no official evidence supporting this idea. Furthermore, subjective factors about the constant power spectrums in the transient condition, which would seem due to the electrons incitement of chaos in the vibration of the nucleus to regulate their movement in this states, appear to suggest there is no disparity in the electron density in reality, and thus QM stops working in a transient crystalline state. In other terms, because the exciton can't be "connected" into the quantum system, as the usual answer to SE(Schrodinger's equation) predicts, it "rolls" so over spectrum ranging of energies to the initial states, as we stated in our subjective reasoning. In photoexcitation, the electrons transition happens at the pivotal moments of the vibrating nucleus, that is, at the instant they stop, according the Franck-Condon rule. This "plausible scenario" in QM allows the nuclear sub - system to be "decided to switch off" from a filled nonlinear dynamic at this time, just as the electronic subsystems is "switched-off" from a filled nonlinear dynamic in a warranted process to isolates the non adiabaticity user in Schrodinger's(S)formula and ignore it in the heat transfer estimate in QM. Different physical facts form the basis of the FCn rule. The first presupposes that quantum theory works in the area of molecule quantum transition (which is, in general, illogical, as already stated). The second proposes that the nuclei spent the majority of their time at the turning point during their classic cycles in an oscillating prospective well. As a result, the quantum shift is sure to happen at these sites, and as a result, it will be horizontal or almost vertical. As a result, the same arpeggiator continues to behave the very same way as a conventional systems (near the bottoms of an oscillations prospective well for

neutrons, where the likelihood of a quantum transformation is marginal) and as a quantum state (nuclei's pivotal moments, where the likelihood of a quantum transformation is maximam). As a result, the oscillator is a QC entity, and the Franck-Condon rule is among the most significant criteria for the development of QC physics.

Divergence of a series of TDPT (time-dependent perturbation theory) in QM for Molecular QM transition:

We can pinpoint the precise instant when QM applied to molecules quantum transition ceases operating using formal QM methods.

$$i\hbar\frac{\partial\psi}{\partial t} = H_{(t)}\psi, \quad H_{(t)} = H_{(0)} + V_{(t)} \quad V_{(t)} = \begin{cases} w_t & if \quad 0\le t\le\pi \\ 0 & t<0,\ t>\pi \end{cases} \tag{1}$$

$$A_{(\eta)}(t) = \sum_{n=0}^{\infty}\frac{\langle f|I_n(t)|l\rangle}{n!} \tag{2}$$

$$I_n(\psi) = \left(\frac{1}{i\hbar}\right)^n \int_0^t dt1 \int_0^t dt2 \dots\dots \int_0^t dtn\breve{W}\,(t1)\,\breve{W}(t2)\dots\dots\dots\dots\breve{W}(tn) \tag{3}$$

$$\breve{W}(t) = e^{\frac{i}{\hbar}H_0 t}\breve{W}(tn)e^{-\frac{i}{\hbar}H_0 t}\frac{i}{\hbar}H_0 t \tag{4}$$

$$\mathfrak{H}_{(\eta)}(\tau) = \left|A_\eta^{(I)}(\tau)\right|^2 = \frac{1}{\hbar^2}\left|\langle f|\ \breve{W}(t)|l\rangle e^{iw\eta t}\right|^2 \tag{5}$$

The Born-Oppenheimer adiabatic approximation:

$$\breve{H} = \breve{T}_e + \breve{T}_n + \mathrm{U(p.q)}, \tag{6}$$

$$\psi_{(q,p)} = \psi_{(q,p)}\phi_{(P)} \tag{7}$$

$$\breve{H}\psi_{(q,p)} = E\psi_{(q,p)} \tag{8}$$

$$\phi\hat{T_e}\psi + \hat{T_N}\psi\phi + U\psi\phi = E\psi\phi \tag{9}$$

$$\hat{L}\psi\phi = \hat{T_N}\psi\phi - \psi\hat{T_N}\phi \tag{10}$$

$$\frac{1}{\psi}\hat{T_e}\psi + U + \frac{1}{\psi\phi}\hat{L}\psi\phi = E - \frac{1}{\phi}\hat{T_N}\phi. \tag{11}$$

$$\left(\hat{T_e} + U + \frac{1}{\phi}\hat{L}\phi\right)\psi = V\psi \tag{12}$$

$$(\hat{T}_N + V)\phi = E\phi \qquad 13$$

$$\left[\hat{T}_e + U(q,p)\right]\psi_f = V_f(p)\psi_f, \qquad 14$$

$$\left[\hat{T}_N + V_f(p)\right]\phi_{fn} = E_{fn}\phi_{fn}, \qquad 15$$

$$V_f^{(1)} = \left\langle\psi_f^{(0)}\middle|\hat{T}_N\middle|\psi_f^{(0)}\right\rangle \qquad 16$$

$$V_f^{(2)} = \sum_{f' \neq f} \frac{\left| \left\langle \psi_{f'}^{(0)} \middle| \hat{T}_N \middle| \psi_f^{(0)} \right\rangle - \sum_p \frac{\hbar^2}{M\phi} \frac{\partial \phi}{\partial p} \left\langle \psi_{f'}^{(0)} \middle| \frac{\partial \psi_f^{(0)}}{\partial p} \right\rangle \right|^2}{V_f^{(0)} - V_{f'}^{(0)}} \quad 17$$

$$\psi_f^{(1)} = \sum_{f' \neq f} \frac{\left\langle \psi_{f'}^{(0)} \middle| \hat{T}_N \middle| \psi_f^{(0)} \right\rangle - \sum_p \frac{\hbar^2}{M\phi} \frac{\partial \phi}{\partial p} \left\langle \psi_{f'}^{(0)} \middle| \frac{\partial \psi_f^{(0)}}{\partial p} \right\rangle}{V_f^{(0)} - V_{f'}^{(0)}} \cdot \psi_{f'}^{(0)} \quad 18$$

Quantum-classical (QC) mechanics of elementary electron transfers in condensed matter

$$\mathrm{H} = -\frac{\hbar^2}{2\mu} \Delta_{\mathbf{q}} + U_1(\mathbf{q}) + U_2(\mathbf{q} - \mathbf{L}) + \sum_l U_l(\mathbf{q}) p_l + \frac{1}{2} \sum_l \omega_l \left(p_l^2 - \frac{\partial^2}{\partial p_l^2} \right) \quad 19$$

$$\mathrm{H}\Psi = E_{\mathrm{H}} \Psi \quad 20$$

$$\Psi(\mathbf{q}, p) = \psi(\mathbf{q}, p) \Phi(p) \quad 21$$

$$\left[-\frac{\hbar^2}{2\mu} \Delta_{\mathbf{q}} + U_1(\mathbf{q}) + U_2(\mathbf{q} - \mathbf{L}) + \sum_l U_l(\mathbf{q}) p_l \right] \psi(\mathbf{q}, p) = E(p) \psi(\mathbf{q}, p) \quad 22$$

$$\hat{L}\Psi \equiv \hat{T}_p \psi \Phi - \psi \hat{T}_p \Phi = -\sum_l \omega_l \left(\frac{\partial \psi}{\partial p_l} \frac{\partial \Phi}{\partial p_l} + \frac{\Phi}{2} \frac{\partial^2 \psi}{\partial p_l^2} \right) \quad 23$$

$$\left(\hat{T}_p = -\frac{1}{2} \sum_l \omega_l \frac{\partial^2}{\partial p_l^2} \right) \text{ in Eq. (20), then}$$

$$\left[E(p) + \frac{1}{2} \sum_l \omega_l \left(p_l^2 - \frac{\partial^2}{\partial p_l^2} \right) \right] \Phi(p) = E_{\mathrm{H}}^{\mathrm{BO}} \Phi(p) \quad 24$$

$$\tilde{U} \equiv \sum_l U_l(\mathbf{q}) \left(p_l - \tilde{p}_l \right) \quad 25$$

$$\left[-\frac{\hbar^2}{2\mu} \Delta_{\mathbf{q}} + U_1(\mathbf{q}) + U_2(\mathbf{q} - \mathbf{L}) + \sum_l U_l(\mathbf{q}) \tilde{p}_l \right] \psi_s(\mathbf{q}) = E_s^0 \psi_s(\mathbf{q}) \quad 26$$

$$\sum_l U_l(\mathbf{q}) \tilde{p}_t$$

$$\tilde{p}_{l2} = -\tilde{p}_{l1} \equiv -\tilde{p}_l \left(\tilde{p}_l < 0 \right) \quad 27$$

$$U_{l2}(\mathbf{q} - \mathbf{L}) = -U_{l1}(\mathbf{q}) \equiv -U_l(\mathbf{q}) \quad 28$$

$$\sum_l U_{l2}(\mathbf{q} - \mathbf{L}) \tilde{p}_{l2} = \sum_l \left[-U_{t1}(\mathbf{q}) \right] \left[-\tilde{p}_{t1} \right] = \sum_l U_{t1}(\mathbf{q}) \tilde{p}_{t1} \equiv \sum_l U_l(\mathbf{q}) \tilde{p}_l$$

$$\int d\mathbf{q} \psi_s * (\mathbf{q}) \tilde{U}(\mathbf{q}, p) \psi(\mathbf{q}) = \int d\mathbf{q} \psi_s^*(\mathbf{q}) \left[\sum_l U_l(\mathbf{q}) \left(p_l - \tilde{p}_l \right) \right] \psi_s(\mathbf{q}) = \sum_l U_{ls} \left(p_l - \tilde{p}_l \right) \quad 29$$

$$U_{ls} \equiv \int d\mathbf{q} U_l(\mathbf{q}) |\psi_s(\mathbf{q})|^2 \quad 30$$

$$E_s(p) = E_s^0 + \tilde{U}_s(p), \tilde{U}_s(p) \equiv \sum_l U_{ls} \left(p_l - \tilde{p}_l \right) \quad 31$$

$$E_s(p) + \frac{1}{2} \sum_l \omega_l \left(p_l^2 - \frac{\partial^2}{\partial p_l^2} \right) = E_s^0 + \sum_l U_{ls} \left(p_l - \tilde{p}_l \right) + \frac{1}{2} \sum_l \omega_l \left(p_l^2 - \frac{\partial^2}{\partial p_l^2} \right) \quad 32$$

$$F_s(p) = E_s^0 + \sum_l U_{ls}\left(p_t - \tilde{p}_t\right) + \frac{1}{2}\sum_l \omega_l p_l^2 \quad 33$$

$$\frac{dF_s}{dp_t} = U_{ls} + \omega_l p_l, \frac{dF_s}{dp_t}\Big|_{p_t=\bar{p}_l} = 0, \frac{d^2F_s}{dp_l^2} = \omega_l > 0$$

$$\bar{p}_l = -\frac{U_{ls}}{\omega_l} \quad 34$$

$$\int d\mathbf{q}|\psi_s(\mathbf{q})|^2 = 1$$

$$\bar{p}_l = \tilde{p}_l \quad 35$$

$$F_s(p)|_{p=\tilde{p}} = E_s^0 + \frac{1}{2}\sum_l \omega_l \tilde{p}_l^2 \equiv E_s^0 + E \equiv J_s \quad 36$$

$$E \equiv \frac{1}{2}\sum_l \omega_l \tilde{p}_l^2 \quad 37$$

$$F_s(p) = J_s + \frac{1}{2}\sum_l \omega_l \left(p_l - \tilde{p}_l\right)^2 \quad 38$$

$$-J_{1,2} + \frac{1}{2}\sum_l \omega_l \left[\left(p_l - \tilde{p}_l\right)^2 - \frac{\partial^2}{\partial p_l^2}\right] \quad 39$$

$$E_{\mathrm{H}}^{\mathrm{BO}} = -J_{1,2} + \sum_l \omega_l \left(m_{l1,2} + \frac{1}{2}\right) \quad 40$$

$$\Phi_{1,2\ldots m_{l1,2}\ldots}(p - \tilde{p}) = \prod_l \varphi_{m_{l1,2}}\left(p_l - \tilde{p}_l\right)$$

$$\varphi_{m_{l1,2}}\left(p_l - \tilde{p}_l\right) = A_{m_{l1,2}} e^{-1/2\left(p_t \mp \tilde{p}_t\right)^2} H_{m_{l1,2}}\left(p_l \mp \tilde{p}_l\right) \quad 41$$

$$\text{Here } H_m(p) = (-1)^m e^{p^2} d^m e^{-p^2}/dp^m$$

$$\Psi_{1,2}^{\mathrm{BO}}(\mathbf{q}, p) = \psi_{1,2}(\mathbf{q})\Phi_{1,2\ldots m_{l1,2}\ldots}(p - \tilde{p}) \quad 42$$

$$\mathrm{H} \equiv \mathrm{H} - \tilde{U} + \tilde{U} \quad 43$$

$$\left(\mathrm{H} - \tilde{U} - E_{\mathrm{H}}\right)\Psi = -\tilde{U}\Psi \quad 44$$

$$\left(\mathrm{H} - \tilde{U} - E_{\mathrm{H}}\right)\tilde{\Psi} = 0 \quad 45$$

$$(\mathrm{H} - E_{\mathrm{H}})G_{\mathrm{H}}\left(\mathbf{q}, \mathbf{q}'; p, p'; E_{\mathrm{H}}\right) = -\Delta\left(\mathbf{q} - \mathbf{q}'\right)\Delta\left(p - p'\right) \quad 46$$

$$\left(\mathrm{H} - \tilde{U} - E_{\mathrm{H}}\right)G\left(\mathbf{q}, \mathbf{q}'; p, p'; E_{\mathrm{H}}\right) = -\Delta\left(\mathbf{q} - \mathbf{q}'\right)\Delta\left(p - p'\right) \quad 47$$

$$G_{\mathrm{H}}\left(\mathbf{q}, \mathbf{q}'; p, p'; E_{\mathrm{H}}\right) = G\left(\mathbf{q}, \mathbf{q}'; p, p'; E_{\mathrm{H}}\right) + \iint d\mathbf{q}_I dp_I G(\mathbf{q}, \mathbf{q}_I; p, p_I; E_{\mathrm{H}})\tilde{U}(\mathbf{q}_I, p_I)G_{\mathrm{H}}\left(\mathbf{q}_I, \mathbf{q}'; p_I, p'; E_{\mathrm{H}}\right) \quad 48$$

$$G_{\mathrm{H}} = G + G\tilde{U}G_{\mathrm{H}} \quad 49$$

$$G_{\mathrm{H}} = G + G\tilde{U}G + G\tilde{U}G\tilde{U}G + \cdots \quad 50$$

$$\Psi(\mathbf{q},p)=\tilde{\Psi}(\mathbf{q},p)+\iint d\mathbf{q}^{'}dp^{'}G\left(\mathbf{q},\mathbf{q}^{'};p,p^{'};E_{\mathrm{H}}\right)\tilde{U}\left(\mathbf{q}^{'},p^{'}\right)\Psi\left(\mathbf{q}^{'},p^{'}\right) \quad 51$$

$$\Psi=\tilde{\Psi}+G\tilde{U}\Psi \quad 52$$

$$\Psi(q,p)=\tilde{\Psi}(q,p)+\iint d\acute{q}\ d\acute{p}\ G(q,\acute{q};p,\acute{p};E_H)\tilde{U}(\acute{q},\acute{p})\Psi(\acute{q},\acute{p}).$$

$$\Psi=\tilde{\Psi}+G\tilde{U}\Psi$$

$$\Psi=\tilde{\Psi}+G\tilde{U}\tilde{\Psi}+G\,\tilde{U}\,G\,\tilde{U}\tilde{\Psi}+\ G\,\tilde{U}\,G\,\tilde{U}\,G\,\tilde{U}\tilde{\Psi}+\ \ldots$$

$$=\tilde{\Psi}+\left(\mathrm{G}+\ G\tilde{U}\mathrm{G}+\ G\tilde{U}G\tilde{U}\mathrm{g}+\ldots\right)\tilde{G}\tilde{\Psi} \quad (53)$$

$$\Psi=\tilde{\Psi}+\ G_H\tilde{U}\tilde{\Psi} \quad (54)$$

$$\mathrm{H}-\tilde{U}=-\frac{\hbar^2}{2\mu}\Delta_{\mathbf{q}}+U_1(\mathbf{q})+U_2(\mathbf{q}-\mathbf{L})+\sum\mathrm{U}_{\ l}\ U_l(\mathbf{q})\tilde{p}_t+\frac{1}{2}\sum\mathrm{U}_{\ l}\ \hbar\omega_l\left(p_t^2-\frac{\partial^2}{\partial p_l^2}\right) \quad (55)$$

$$\tilde{\Psi}(\mathbf{q},p)=\psi(\mathbf{q})\Phi_0(p) \quad (56)$$

$$\Psi=G_{\mathrm{H}}\tilde{U}\tilde{\Psi}. \quad (57)$$

$$\Psi_1=G_{\mathrm{H}}\tilde{U}\Psi_1^{\mathrm{BO}} \quad (58)$$

$$G\equiv G\left(\mathbf{q},\mathbf{q}^{'};p,p^{'};\mathbf{H}-\tilde{U}\right)=\sum_s\frac{\Psi_s(\mathbf{q},p)\Psi_s^*\left(\mathbf{q}^{'},p^{'}\right)}{E_{\mathrm{H}}^{\mathrm{BO}}-\left(E_s(p)-\tilde{U}(p)\right)-i\gamma} \quad (59)$$

$$\tilde{U}G\sim\frac{\tilde{U}}{\gamma}\sim\frac{\hbar\omega_1}{\gamma}<<1. \quad (60)$$

$$G>>G\tilde{U}G>>G\tilde{U}G\tilde{U}G>>\cdots \quad (61)$$

$$G_{\mathrm{H}}\approx G. \quad (62)$$

$$\Psi_1\approx G\tilde{U}\Psi_1^{\mathrm{BO}} \quad (63)$$

$$A_{12}=\langle\Psi_2(\mathbf{q}-\mathbf{L},p)|\mathrm{W}|\Psi_1(\mathbf{q},p)\rangle \quad (64)$$

$$(\bar{m}_1\hbar\omega_t/\gamma)^2<<1 \quad (65)$$

$$(k_{\mathrm{B}}T/\gamma)^2<<1. \quad (66)$$

$$\frac{\hbar\omega}{\gamma}<<1 \quad (67)$$

4- The simplest electron-phonon Green's function:

$$G\left(\mathbf{q},\mathbf{q}^{'};\mathbf{L};p,p^{'};E_{\mathrm{H}}^{\mathrm{BO}}\right)=\sum_{\ldots m_t\ldots}G_e\left(\mathbf{q},\mathbf{q}^{'};\mathbf{L};\tilde{p};E_{\mathrm{H}}^{\mathrm{BO}}-\varepsilon_{\ldots m_t\ldots}\right)\Phi_{0\ldots m_t\ldots}(p)\Phi_{0\ldots m_t\ldots}\left(p^{'}\right) \quad (68)$$

$$G_e\left(\mathbf{q},\mathbf{q}^{'};\mathbf{L};\tilde{p};E_{\mathrm{H}}^{\mathrm{BO}}-\varepsilon_{\ldots m_1\ldots\ldots}\right)=\sum_s\frac{\psi_s(\mathbf{q};\mathbf{L};\tilde{p})\psi_s\ \ ^*\left(\mathbf{q}^{'};\mathbf{L};\tilde{p}\right)}{\left(E_{\mathrm{H}}^{\mathrm{BO}}-\varepsilon_{\ldots m_t\ldots}\right)-E_s(\mathbf{L};\tilde{p})-i\gamma} \quad (69)$$

$$\varepsilon_{\ldots m_l \ldots} \equiv \sum_i \hbar\omega_\iota \left(m_\iota + \tfrac{1}{2}\right) \tag{70}$$

$$G_e = G^{(\text{free})} - G^{(\text{free})}\hat{T}G^{(\text{free})} \tag{71}$$

$$G^{(\text{free})} \equiv G^{(\text{free})}(\mathbf{q}, \mathbf{q}^{'}; k) = \frac{\mu}{2\pi\hbar^2}\frac{\exp\left(\pm ik|\mathbf{q}-\mathbf{q}^{'}|\right)}{|\mathbf{q}-\mathbf{q}^{'}|} \tag{72}$$

$$E_{\mathrm{H}}^{\mathrm{BO}} - \varepsilon_{\ldots m_t \ldots} - i\gamma = -(J_1 + \hbar\omega_1 + i\gamma) \tag{73}$$

$$\omega_1 \equiv \sum_t \omega_l (m_t - m_{t1}). \tag{74}$$

$$k = \pm\frac{i[2\mu(J_1 + \hbar\omega_1 + i\gamma)]^{\frac{1}{2}}}{\hbar}. \tag{75}$$

$$G_e \cong G^{(\text{free})}. \tag{76}$$

$$G_e(\mathbf{q}, \mathbf{q}^{'}; \alpha) = \frac{\mu}{2\pi\hbar^2}\frac{\exp\left(-\alpha|\mathbf{q}-\mathbf{q}^{'}|\right)}{|\mathbf{q}-\mathbf{q}^{'}|} \tag{77}$$

$$\alpha \equiv \alpha(\ldots m_l \ldots) \equiv \alpha(\omega_1) = \frac{[2\mu(J_1 + \hbar\omega_1 + i\gamma)]^{\frac{1}{2}}}{\hbar} \tag{78}$$

$$G(\mathbf{q}, \mathbf{q}^{'}; p, p^{'}) = \sum_{\ldots m_l \ldots} G_e[\mathbf{q}, \mathbf{q}^{'}; \alpha(\ldots m_l \ldots)]\Phi_{0\ldots m_\ell \ldots}(p)\Phi_{0\ldots m_t \ldots}(p^{'}) \tag{79}$$

$$A_{12} = \sum_l \sum_{m_t \ldots} A_l[J_1 + \sum_t \hbar\omega_t(m_t - m_{t1}); L; \tilde{p}]\frac{o(m_l, m_{t1})}{r(m_l, m_{l1})}\prod_l r(m_{l2}, m_t)r(m_t, m_{t1}) \tag{80}$$

$$A_l[J_1 + \sum_t \hbar\omega_t(m_t - m_{t1}); L; \tag{81}$$

$$\prod_l r(m_l, m_{l1,2}) \equiv \prod_l \int \varphi_{m_l}(p_l)\varphi_{m_{l1,2}}(p_l - \tilde{p_l})dp_l = \int \Phi_{0\ldots m_l \ldots}(p)\Phi_{1,2\ldots m_{l1,2}\ldots}(p - \tilde{p})dp \tag{82}$$

$$o(m_l, m_{l1}) \equiv -\int \varphi_{m_{l1}}(p_l^{'} - \tilde{p_l})(p_l^{'} - \tilde{p_l})\varphi_{m_l}(p_l^{'})dp_l^{'} \tag{83}$$

$$\psi_1(\mathbf{q}^{'}) = \left(\frac{\alpha_1}{2\pi}\right)^{1/2}\frac{\exp(-\alpha_1|\mathbf{q}^{'}|)}{|\mathbf{q}^{'}|} \tag{84}$$

$$\psi_2 * (\mathbf{q}) = \left(\frac{\alpha_2}{2\pi}\right)^{1/2}\frac{\exp(-\alpha_2|\mathbf{q}-\mathbf{L}|)}{|\mathbf{q}-\mathbf{L}|} \tag{85}$$

Where

$$\alpha_{1,2} = \frac{[2\mu(J_{1,2}-E)]^{1/2}}{} \tag{86}$$

$$A_l = -\frac{\mu(\alpha_1\alpha_2)^{1/2}}{(2\pi)^2}\,\omega_l\tilde{p}_{l1}\int I(|\mathbf{q}|)\exp(-\alpha_2|\mathbf{q}-\mathbf{L}|)d\mathbf{q} \tag{87}$$

$$I(|\mathbf{q}|) = \frac{4\pi[\exp(-\alpha|\mathbf{q}|)-\exp(-\alpha_1|\mathbf{q}|)]}{(\alpha_1^2-\alpha^2)|\mathbf{q}|} \tag{88}$$

$$A_l = c_{12}\omega_l\tilde{p}_{l1}G^{\mathrm{E}} \tag{89}$$

Where

$$c_{12} = -\frac{\delta\mu\alpha_2(\alpha_1\alpha_2)^{1/2}}{} \quad 90$$

$$G^{\mathrm{E}} = G^{\mathrm{E}}(\alpha, L) = \frac{1}{L}\left[\frac{\exp(-\alpha L)+f(\alpha,L)}{(\alpha_1^2-\alpha^2)(\alpha_2^2-\alpha^2)^2}\right] \quad 91$$

$$f(\alpha, L) \equiv \left\{\left[1+\frac{(\alpha_2^2-\alpha_1^2)L}{2\alpha_2}\right]\exp(-\alpha_2 L) - \exp(-\alpha_1 L)\right\}\frac{(\alpha_2^2-\alpha^2)^2}{(\alpha_2^2-\alpha_1^2)^2} - \left[\frac{L}{2\alpha_2}\exp(-\alpha_2 L)\right](\alpha_2^2-\alpha^2) - \exp(-\alpha_2 L), \quad 92$$

$$\varepsilon = \frac{4\pi^2 q^2 M_{\mathrm{A}}\Omega}{3\,cn_{\mathrm{ref}}}K \quad 93$$

$$\sum_l \omega_l(m_{l2}-m_{l1}) = \omega_{12} \quad 94$$

$$\Omega = J_1 - J_2 + \omega_{12} \quad 96$$

$$\sum_l \omega_l(m_l - m_{l1}) = \omega_1 \quad 74(a)$$

$$A_{12} = c_{12}\sum_l \omega_l\tilde{p}_{l1}\sum_{\omega_1=-\infty}^{\infty} G^{\mathrm{E}}(\omega_1, L)P_l(m_{l2}, m_{l1}; \omega_1) \quad 97$$

$$P_l(m_{l2}, m_{l1}; \omega_1) \equiv \sum_{\ldots m_l \ldots}\frac{o(m_l, m_{l1})}{r(m_l, m_{l1})}\prod_l r(m_{l2}, m_l)r(m_l, m_{l1})\Delta\left[\omega_1 - \sum_l \omega_l(m_l - m_{l1})\right], \quad 98$$

5-The general expression for the rate constant of elementary electron photo-transfers. The technique of generating functions:

$$P_l^{\mathrm{FC}}(m_{l2}, m_{l1}) = \frac{o(m_{l2}, m_{l1})}{r(m_{l2}, m_{l1})}\prod_l r(m_{l2}, m_{l1}), \quad 99$$

$$A_{12} = c_{12}G^{\mathrm{E}}(\omega_1 = \text{ constant }, L)\sum_l \omega_l\tilde{p}_{l1}P_l^{\mathrm{FC}}(m_{l2}, m_{l1}) \quad 100$$

$$f(w) = \sum_{m=-\infty}^{\infty} b_m(w-w_0)^m, b_m = \frac{1}{2\pi i}\oint\frac{f(\zeta)}{(\zeta-w_0)^{m+1}}d\zeta \quad 101$$

$$rr(m_{l2}, m_{l1}; u) \equiv r(m_{l2}, m_{l1})r(m_{l1}, m_{l1}) + u^{\omega_l}r(m_{l2}, m_{l1}+1)r(m_{l1}+1, m_{l1}) + \cdots + u^{-\omega_l}r(m_{l2}, m_{l1}-1)r(m_{l1}-1, m_{l1}) + \cdots \quad 102$$

$$ro(m_{l2}, m_{l1}; u) \equiv r(m_{l2}, m_{l1})o(m_{l1}, m_{l1}) + u^{\omega_l}r(m_{l2}, m_{l1}+1)o(m_{l1}+1, m_{l1}) + \cdots + u^{-\omega_l}r(m_{l2}, m_{l1}-1)o(m_{l1}-1, m_{l1}) + \cdots \quad 103$$

$$P_l(m_{l2}, m_{l1}; \omega_1) = \frac{1}{2\pi i}\oint\frac{du}{u^{\omega_1+1}}\frac{\mathrm{ro}(m_{l2}, m_{l1}; u)}{rr(m_{l2}, m_{l1}; u)}\prod_l rr(m_{l2}, m_{l1}; u) \quad 104$$

$$K = c_{12}^2\sum_{\omega_1=-\infty}^{\infty} G^{\mathrm{E}}(\omega_1, L)\sum_{\omega_1'=-\infty}^{\infty} G^{\mathrm{E}*}(\omega_1', L)\sum_l \omega_l\tilde{p}_{l1}\sum_{l'}\omega_{l'}\tilde{p}_{l'1}Av(m_{l1})\sum_{\ldots m_{l2}\ldots} P_l(m_{l2}, m_{l1}; \omega_1)P_t(m_{l2}, m_{l1}; \omega_1')\Delta\left[\omega_{12} - \sum_l \omega_l(m_{l2}-m_{l1})\right], \quad 105$$

$$P_{l'}(m_{l2}, m_{l1}; \omega_1') = \frac{1}{2\pi i}\oint\frac{dv}{v^{\omega_1'+1}}\frac{\mathrm{ro}(m_{l'2}, m_{l'1}; v)}{\mathrm{rr}(m_{l'2}, m_{l'1}; v)}\prod_l rr(m_{l2}, m_{l1}; v) \quad 106$$

$$Av(m_{lI})\sum_{\dots m_{l2}\dots} P_l(m_{l2},m_{lI};\omega_I)P_{l'}(m_{l2},m_{lI};\omega'_I)\Delta\left[\omega_{I2}-\sum_l \omega_l(m_{l2}-m_{lI})\right] \quad 107$$

$$\sum_l \omega_l\tilde{p}_{lI}\sum_{l'}\omega_{l'}\tilde{p}_{l'I}R_{l,l'}(\omega_I,\omega'_I;\omega_{I2}) \equiv \phi(\omega_I,\omega'_I;\omega_{I2}) \quad 108$$

$$K \equiv K(\omega_{I2}) = c_{I2}^2$$

$$\times\sum_{\omega_I=-\infty}^{\infty} G^{\mathrm{E}}(\omega_I,L)\sum_{\omega'_I=-\infty}^{\infty} G^{\mathrm{E}}*(\omega'_I,L)\sum_l \omega_l\tilde{p}_{lI}\sum_{l'}\omega_{l'}\tilde{p}_{l'I}R_{l,l'}(\omega_I,\omega'_I;\omega_{I2}) \quad 109$$

$$R_{l,l}(\omega_I,\omega'_I;\omega_{I2}) = Av(m_{lI})\frac{1}{(2\pi i)^2}\oint\frac{du}{u^{\omega_I+1}}\oint\frac{dv}{v^{\omega'_I+1}}$$

$$\sum_{\dots m_{l2}\dots}\Delta\left[\omega_{I2}-\sum_t \omega_t(m_{l2}-m_{lI})\right]\frac{ro(m_{l2},m_{lI};u)ro(m_{l'2},m_{l'I};v)}{rr(m_{l2},m_{lI};u)rr(m_{l'2},m_{l'I};v)}\prod_t rr(m_{l2},m_{lI};u)rr(m_{l2},m_{lI};v) \quad (110)$$

$$R_{l,l}(\omega_I,\omega'_I;\omega_{I2}) = Av(m_{lI})\frac{1}{(2\pi i)^3}\oint\frac{du}{u^{\omega_I+1}}\oint\frac{dv}{v^{\omega'_I+1}}\oint\frac{dw}{w^{\omega_{I2}+1}}\mathrm{rorr}(m_{lI};u,v,w)\,\mathrm{rrro}(m_{l'I};u,v,w)\prod_t rrrr(m_{lI};u,v,w), \quad (111)$$

$$\mathrm{rrrr}(m_{lI};u,v,w) \equiv rr(m_{lI},m_{lI};u)rr(m_{lI},m_{lI};v) + w^{\omega_l}\,\mathrm{rr}(m_{lI}+1,m_{lI};u)rr(m_{lI}+1,m_{lI};v)+\cdots$$
$$+ w^{-\omega_l}rr(m_{lI}-1,m_{lI};u)rr(m_{lI}-1,m_{lI};v)+\cdots, \quad (112)$$

$$\mathrm{rorr}(m_{lI};u,v,w)\,\mathrm{rrrr}(m_{lI};u,v,w) \equiv o(m_{lI},m_{lI};u)\,\mathrm{rr}(m_{lI},m_{lI};v) + w^{\omega_l}\,\mathrm{ro}(m_{lI}+1,m_{lI};u)\,\mathrm{rr}(m_{lI}+1,m_{lI};v)+\cdots$$
$$+ w^{-\omega_l}\,\mathrm{ro}(m_{lI}-1,m_{lI};u)rr(m_{lI}-1,m_{lI};v)+\cdots \quad (113)$$

$$\mathrm{rrro}(\ ;\ ,\ ,\ )\,\mathrm{rrrr}(\ ;\ ,\ ,\ )$$
$$\equiv \mathrm{rr}(m_{l'I},m_{l'I};u)\,\mathrm{ro}(m_{l'I},m_{l'I};v) + w^{\omega_{l'}}\,\mathrm{rr}(m_{l'I}+1,m_{l'I};u)\,\mathrm{ro}(m_{l'I}+1,m_{l'I};v)+\cdots$$
$$+ w^{-\omega_{l'}}\,\mathrm{rr}(m_{l'I}-1,m_{l'I};u)\,\mathrm{ro}(m_{l'I}-1,m_{l'I};v)+\cdots \quad (114)$$

6-The case of non-local phonons:

$$R_{l,l}(\omega_I,\omega'_I;\omega_{I2}) = Av(m_{lI})\frac{1}{(2\pi i)^3}\oint\frac{du}{u^{\omega_I+1}}\oint\frac{dv}{v^{\omega'_I+1}}\oint\frac{dw}{w^{\omega_{I2}+1}}\mathrm{roro}(m_{lI};u,v,w)\prod_l rrrr(m_{lI};u,v,w) \quad (115)$$

$$\mathrm{roro}\,(m_{lI};u,v,w)\mathrm{rrrr}\,(m_{lI};u,v,w) \equiv \mathrm{ro}\,(m_{lI},m_{lI};u)\mathrm{ro}\,(m_{lI},m_{lI};v)$$
$$+w^{\omega_l}\mathrm{ro}\,(m_{lI}+1,m_{lI};u)\mathrm{ro}\,(m_{lI}+1,m_{lI};v)+\cdots \quad (116)$$
$$+w^{-\omega_l}\mathrm{ro}\,(m_{lI}-1,m_{lI};u)\mathrm{ro}\,(m_{lI}-1,m_{lI};v)+\cdots$$

$$K = c_{I2}^2\sum_{\omega_I=-\infty}^{\infty} G^{\mathrm{E}}(\omega_I,L)\sum_{\omega'_I=-\infty}^{\infty} G^{\mathrm{E}}*(\omega'_I,L)\frac{1}{(2\pi i)^3}\oint\frac{du}{u^{\omega_I+1}}\oint\frac{dv}{v^{\omega'_I+1}}\oint\frac{dw}{w^{\omega_{I2}+1}}Av(m_I)[P(m_I;u,v,w)R(m_I;u,v,w)] \quad (117)$$

$$P(m_I;u,v,w) \equiv \sum_l\sum_{l'\neq l}\omega_l\omega_{l'}\tilde{p}_{lI}\tilde{p}_{l'I}\mathrm{rorr}\,(m_{lI};u,v,w)\mathrm{rrro}\,(m_{l'I};u,v,w)$$
$$+\sum_l \omega_l^2\tilde{p}_{lI}^2\mathrm{roro}\,(m_{lI};u,v,w) \quad (118)$$

$$R(m_I;u,v,w) \equiv \prod_l \mathrm{rrrr}(m_{lI};u,v,w) \quad (119)$$

$$\phi(\omega_I,\omega'_I;\omega_{I2}) \equiv \phi(\omega_I,\omega'_I;T;\omega_{I2})$$
$$= \frac{1}{(2\pi i)^3}\oint\frac{du}{u^{\omega_I+1}}\oint\frac{dv}{v^{\omega'_I+1}}\oint\frac{dw}{w^{\omega_{I2}+1}}Av(m_I)\times[P(m_I;u,v,w)R(m_I;u,v,w)] \quad (120)$$

$$Av(m_I)[P(m_I;u,v,w)R(m_I;u,v,w)] \quad (121)$$

$$\tilde{p}_l \sim M^{-1/2} \quad (122)$$

$$r(m_{lI},m_{lI}) = 1-\frac{\tilde{p}_l^2}{2}\left(m_{lI}+\frac{1}{2}\right)+\cdots, r(m_{lI}+1,m_{lI}) = \tilde{p}_l\sqrt{\frac{m_{lI}+1}{2}}+\cdots, r(m_{lI}-1,m_{lI}) = -\tilde{p}_l\sqrt{\frac{m_{lI}}{2}}+\cdots \quad (123)$$

$$o(m_{lI},m_{lI}) = \frac{\tilde{p}_l}{2}+\cdots, o(m_{lI}+1,m_{lI}) = \sqrt{\frac{m_{lI}+1}{2}}+\cdots o(m_{lI}-1,m_{lI}) = \sqrt{\frac{m_{lI}}{2}}+\cdots \quad (124)$$

$$\mathrm{rrrr}(m_{lJ};u,v,w) = 1-\left(\tilde{p}_{l1}^2+\tilde{p}_{l2}^2\right)\left(m_{lJ}+\frac{1}{2}\right)+\frac{1}{2}\tilde{p}_{l1}^2[(m_{lJ}+1)(uvw)^{\omega_l}+m_{lJ}(uvw)^{-\omega_l}]+\frac{1}{2}\tilde{p}_{t2}^2[(m_{lJ}+1)w^{\omega_l}+m_{lJ}w^{-\omega_l}]$$
$$-\frac{1}{2}\tilde{p}_{ll}\tilde{p}_{l2}[(m_{lJ}+1)(u^{\omega_l}+v^{\omega_t})(w^{\omega_l}-1)+m_{lJ}(u^{-\omega_t}+v^{-\omega_t})(w^{-\omega_l}-1)] \quad (125)$$

$$\mathrm{rorr}\,(m_{lJ};u,v,w)\mathrm{rrrr}\,(m_{lJ};u,v,w) = \frac{\tilde{p}_{lJ}}{2}[1+(m_{lJ}+1)(uvw)^{\omega_l}-m_{lJ}(uvw)^{-\omega_l}]$$
$$-\frac{\tilde{p}_{l2}}{2}[(m_{lJ}+1)u^{\omega_l}(w^{\omega_l}-1)-m_{lJ}u^{-\omega_l}(w^{-\omega_l}-1)] \quad (126)$$

$$\mathrm{rrro}(\ _J;\ ,\ ,\ )\ \mathrm{rrrr}(\ _J;\ ,\ ,\ )$$
$$=\frac{\tilde{p}_{lJ}}{2}[1+(m_{lJ}+1)(vuw)^{\omega_l}-m_{lJ}(vuw)^{-\omega_l}]-\frac{\tilde{p}_{l2}}{2}[(m_{lJ}+1)v^{\omega_l}(w^{\omega_l}-1)-m_{lJ}v^{-\omega_l}(w^{-\omega_l}-1)]$$
$$=\mathrm{rorr}(m_{lJ};v,u,w)\,\mathrm{rrrr}(m_{lJ};v,u,w)=\mathrm{rorr}(m_{lJ};v,u,w)\,\mathrm{rrrr}(m_{lJ};u,v,w), \quad (127)$$

$$\mathrm{roro}(m_{lJ};v,u,w)\,\mathrm{rrrr}(m_{lJ};u,v,w)=\frac{1}{2}[(m_{lJ}+1)(uvw)^{\omega_l}+m_{lJ}(uvw)^{-\omega_l}] \quad (128)$$

$$\bar{\mathrm{m}}_{lJ,lJ}=\left[\exp\left(\omega_{l,l}/k_{\mathrm{B}}T\right)-1\right]^{-1} \quad (129)$$

$$K=c_{J2}^2\sum_{\omega_J=-\infty}^{\infty}\sum_{\omega_J'=-\infty}^{\infty}G^{\mathrm{E}}(\omega_J,L)G^{\mathrm{E}*}\left(\omega_J',L\right)\frac{1}{(2\pi i)^3}\oint\frac{du}{u^{\omega_J+1}}\oint\frac{dv}{v^{\omega_J'+1}}\oint\frac{dw}{w^{\omega_{J2}+1}}P(\bar{\mathrm{m}}_J;u,v,w)R(\bar{\mathrm{m}}_J;u,v,w) \quad (130)$$

$$R\left(\bar{m}_J;u,v,w\right)=\exp\{-\sum_l\tilde{p}_l^2(2\bar{\mathrm{m}}_{lJ}+1)$$
$$+\frac{1}{2}\sum_l\tilde{p}_l^2[(\bar{\mathrm{m}}_{lJ}+1)(u^{\omega_l}v^{\omega_l}+1)w^{\omega_l}+\bar{\mathrm{m}}_{lJ}(u^{-\omega_l}v^{-\omega_l}+1)w^{-\omega_l}]\}, \quad (131)$$

$$P(\bar{\mathrm{m}}_J;u,v,w)=\frac{1}{4}\left\{\sum_l\omega_l\tilde{p}_l^2[1+(\bar{\mathrm{m}}_{lJ}+1)(uvw)^{\omega_l}-\bar{\mathrm{m}}_{lJ}(uvw)^{-\omega_l}]\right\}$$
$$+\frac{1}{2}\sum_l\omega_l^2\tilde{p}_l^2[(\bar{\mathrm{m}}_{lJ}+1)(uvw)^{\omega_l}+\bar{\mathrm{m}}_{lJ}(uvw)^{-\omega_l}].^2 \quad (132)$$

7-The analytical result for the shape of the optical absorption band:

$$G^{\mathrm{E}}(J_J+\ \omega_J;L)\approx G^{\mathrm{E}}(J_J;L)\exp(-t\omega_J) \quad (133)$$

$$t=-\left[\partial\ln\ G^{\mathrm{E}}(J_J+\ \omega_J;L)/\ \partial\omega_J\right]_{\omega_J=0} \quad (134)$$

$$K=c_{J2}^2\left|G^{\mathrm{E}}(J_J;L)\right|^2\frac{1}{2\pi i}\oint\frac{dw}{w^{\omega_{J2}+1}}P[\bar{\mathrm{m}}_J;u=\exp(-t),v$$
$$=\exp(-t),w]R[\bar{\mathrm{m}}_J;u=\exp(-t),v=\exp(-t),w] \quad (135)$$

$$\omega_{l,l}<<|\omega_{J2}| \quad (136)$$

$$K=c_{J2}^2\left|G^{\mathrm{E}}(J_J;L)\right|^2P[\bar{\mathrm{m}}_J;u=\exp(-t),v=\exp(-t),w=1]\frac{1}{2\pi i}\oint\frac{dw}{w^{\omega_{J2}+1}}R[\bar{\mathrm{m}}_J;u=\exp(-t),v=\exp(-t),w] \quad (137)$$

$$\exp\left(Az+\frac{B}{z}\right)=\sum_{n=-\infty}^{\infty}z^n\left(\frac{A}{B}\right)^{\frac{n}{2}}I_n\left(2\sqrt{AB}\right) \quad (138)$$

$$K=c_{J2}^2\left|G^{\mathrm{E}}(J_J;L)\right|^2P\left[\bar{m}_J;u=\exp(-t),v=\exp(-t),w=1\right]\exp\left[-\frac{2E}{\omega}\mathrm{cth}\,\beta_T+(\beta_T-t)\frac{\omega_{J2}}{\omega}\right]I_{\frac{\omega_{J2}}{\omega}}\left(\frac{2\,\mathrm{Ech}\,t}{\omega\,\mathrm{sh}\,\beta_T}\right), \quad (139)$$

$$I_\kappa(u)\approx\frac{1}{\sqrt{2\pi u}}\exp\left(u-\frac{\kappa^2}{2u}\right),u>>1,\kappa\le u \quad (140)$$

$$K = K_0 \exp(Y) \tag{141}$$

$$Y = \frac{1}{2}\ln\left(\frac{\omega\tau\sinh\ \beta_T}{4\pi\cosh\ t}\right) - \frac{2}{\omega\tau}\left(\coth\ \beta_T - \frac{\cosh\ t}{\sinh\ \beta_T}\right) + (\beta_T - t)\frac{1}{\omega\tau\Theta} - \frac{\sinh\ \beta_T}{4\omega\tau\Theta^2\cosh\ t} \tag{142}$$

$$1 << \frac{1}{\omega\tau\Theta} \leq \frac{2\cosh\ t}{\omega\tau\sinh\ \beta_T} \tag{143}$$

Where

$$t = \frac{\omega\tau_e}{\theta}\left[\frac{AC + BD}{A^2 + B^2} + \frac{2\Theta(\Theta - 1)}{(\Theta - 1)^2 + (\Theta/\theta_0)^2} + \frac{\theta_0^2}{\theta_0^2 + 1}\right] \tag{144}$$

$$|\theta_0| >> \frac{E}{2J_1} \tag{145}$$

$$\theta \equiv \frac{\tau_e}{\tau} = \frac{LE}{\sqrt{2J_1/m}}, \Theta \equiv \frac{\tau'}{\tau} = \frac{E}{\Delta}, \theta_0 \equiv \frac{\tau_0}{\tau} = \frac{E}{\gamma} \tag{146}$$

$$\tau_e = \frac{L}{\sqrt{2J_1/m}}, \tau = \frac{}{E}, \tau' = \frac{}{\Delta}, \tau_0 = \frac{}{\gamma} \tag{147}$$

$$A = \cos\left(\frac{\theta}{\theta_0}\right) + \Lambda + \left(\frac{1}{\theta_0}\right)^2 \nu, B = \sin\left(\frac{\theta}{\theta_0}\right) + \frac{1}{\theta_0}\mu \tag{148}$$

$$C = \theta\left[\cos\left(\frac{\theta}{\theta_0}\right) - \frac{1 - \xi^2}{2\theta_0}\sin\left(\frac{\theta}{\theta_0}\right)\right] + \mu \tag{149}$$

$$D = \theta\left[\sin\left(\frac{\theta}{\theta_0}\right) + \frac{1 - \xi^2}{2\theta_0}\cos\left(\frac{\theta}{\theta_0}\right)\right] - \frac{2}{\theta_0}\nu, \tag{150}$$

$$\xi \equiv \left(1 - \frac{E}{J_1}\right)^{1/2} (J_1 > E \text{ by definition }) \tag{151}$$

$$\Lambda = -(\Theta - 1)^2\varepsilon + \left[\frac{(\Theta - 1)\theta}{\rho} + \Theta(\Theta - 2)\right]\varepsilon^{\frac{1-\rho}{1-\xi}} \tag{152}$$

$$\mu = 2\Theta(\Theta - 1)\varepsilon - \left[\frac{(2\Theta - 1)\theta}{\rho} + 2\Theta(\Theta - 1)\right]\varepsilon^{\frac{1-\rho}{1-\xi}} \tag{153}$$

$$\nu = \Theta\left[\Theta\varepsilon - \left(\frac{\theta}{\rho} + \Theta\right)\varepsilon^{\frac{1-\rho}{1-\xi}}\right] \tag{154}$$

$$\varepsilon \equiv \exp\left(\frac{2\theta}{1 + \xi}\right), \rho \equiv \sqrt{\xi^2 + \frac{1 - \xi^2}{\Theta}} \tag{155}$$

$$K_0 = K_0^e K_0^p \tag{156}$$

$$K_0^e = \frac{2\tau^3 J_1}{m} \frac{(A^2 + B^2)\rho^3 \Theta^4 \xi}{\theta^2 \left[(\Theta - 1)^2 + \left(\frac{\Theta}{\theta_0}\right)^2\right]^2 \left[1 + \left(\frac{1}{\theta_0}\right)^2\right]} \exp\left(-\frac{4\theta}{1 - \xi^2}\right) \quad (157)$$

$$K_0^p = \frac{1}{\omega\tau}\left[1 + \frac{\sinh(\beta_T - 2t)}{\sinh \beta_T}\right]^2 + \frac{\cosh(\beta_T - 2t)}{\sinh \beta_T} \quad (158)$$

$$\tau_e = \frac{L}{\sqrt{2J_1/m}} \quad (159)$$

$$\tau = \frac{}{E} \quad (160)$$

$$(2\tau_e)^{-1} = \tau^{-1} \quad (161)$$

$$\frac{K_0^e(\Theta = 1, \theta_0 \to \infty)}{2\tau^3 J_1/m} = \frac{\xi}{\theta^2}\left[\exp\left(\frac{2\theta}{1 + \xi}\right) - \frac{\theta^2}{2} - \theta - 1\right]^2 \exp\left(-\frac{4\theta}{1 - \xi^2}\right) \quad (162)$$

8-Limit to standard result:

$$K = \frac{a^2}{\sqrt{4\pi\lambda_r k_B T}} \exp\left(-\frac{2L}{a}\right) exp\left[-\frac{(\Delta - \lambda_r)^2}{4\lambda_r k_B T}\right] \quad (163)$$

Conclusion

The concept of quantum transition is based on the completion of a succession of time dependent (TD) perturbation theories in quantum theory. This sequence coheres in atomic and nuclear mechanics because quantum transfers have no dynamic by nature. The kinetics of "quantum" transition, which are dictated by the coupled motion of a lightweight electron and very massive nuclei, are inherent by nature in chemical and molecular physics, and the sequence of TD perturbation theory become unique. The dynamics problem for reference frames in the QM approach is an exception, because the electronic subsystems is "removed" from the main dynamic system and hence is not physically filled: it just produces an electromotive force wherein the nuclei oscillation. There are two approaches to get rid of the abovementioned singularities. The first way involved adding an additional assumption into molecule quantum theory in the shape of the Franck-Condon rule, which use the isothermal approach. The author developed the second strategy, which involved injecting chaos to dampen the unique dynamics of the bonding movement of nuclei and electron in the intermediary state of molecular "quantum" transition. Dozy pandemonium is a type of chaos that occurs solely during molecular quantum events. Technically, damping is accomplished by substituting a finite quantity for an endlessly small imagined additive in the spectrum form of the state's full Green's functional. In the molecule transient stage, damping chaos leads to energy spectrum consistency, which is an indication of classical physics. However, in the adiabatic approach, the molecule's starting and end states follow quantum physics. Quantum-classical mechanics is a branch of molecule quantum theory that consider dynamics of the transitory molecular state of "quantum" transition. Dozychaos technicians of primary education electron carriers in crystalline materials, which is the easiest case of DC (dozy chaos) mechanical systems, and its implementations to a broad variety of cases, including the absorption spectrum in dyes of polymethine and their collection, have previously demonstrated the effectiveness of the dampers for the above said beginning of the universe. This study explains the elementary electron DC mechanics exchanges in a systematic way. The key results of its implementations are also discussed, as they were in the introductory.

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