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QUANTUM FIELD THEORETIC AND FEYNMAN DIAGRAM BASED QUANTUM DYNAMIC MODELING OF NANOSTRUCTURED MATERIALS FOR ELECTRONIC DEVICES

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Abstract: We present in this paper first a brief quantum dynamical reviews of some functionally important nano-structured materials for quantum electronic devices. The energy quantization of nanostructures can be described by various quantum mechanical methods like Schrodinger differential wave equation and other approaches in. terms of wave functions in complex vector (Hilbert) space.

Further to understand the quantum behavior of electrons and other charge carriers including elementary excitations or Quasi Particle (QP)and Collective Excitations (CE) in nanostructures, we need the best generalized accurate way to use the language of quantum field theory (QFT) with Feynman Diagram (FD) for quantum electronic devices. To explain quantum confinement effect (QCE) and other important quantum effects for nano quantum materials utilized for quantum electronic devices, QFT with FD provides a very powerful tool for modelling nanostructured quantum materials in terms of relativistic quantum fields in complex vector (Hilbert) Space. Actually, particles are minimum quantum of oscillations in the corresponding quantum fields according to QFT. The quantum interactions among quantum particles are really the interactions among corresponding relativistic quantum fields with the exchange of Quasi Particle (QP) and Collective Excitations (CE) within the regime of QFT with FD.

Keywords: Collective Excitations, Energy Quantization, Feynman diagrams, Hilbert space, Nano structures, Quantum Dynamics, Quasi particle, Quantum Field Theory, Quantum Oscillations, Quantum Confinement Effect, Relativistic Quantum Fields, Vector Space.

I. INTRODUCTION

To understand the quantum dynamics of nano structures, we use common conventional methods of quantum mechanics like Schrodinger differential wave equation or Heisenberg's matrix method or Dirac's Clifford (geometric) algebraic methods in Hilbert Space. Symmetry effects and hence conservation principles (Noether's theorem) are also very important in the systematic quantum dynamical analysis of atoms, molecules, nano particles or nano composites. It is observed now in scientific research of nano-quantum materials in such a stage that the individual electrons, atoms or molecule activating quantum mechanism [1] fall under observation and sometimes the thrust on materials approaches the single electron or multi electron cloud, bosons, fermions, photons or other elementary particles/quasi particles [2].

Quantum electronics or spinotronics devices with quantum nano-materials are on the basis of energy transfer in terms of spin current instead of conducted electronic current which promotes fundamental new avenues for applying these nano objects into nano electro-mechanical system, nano resonators, nano motors, nano thermal sensors, microprocessors, memory cards as in quantum computers, sensors. Spinotronics also helps in miniaturization (ULSI) of integrated circuits (IC) for quantum computers minimizing heat dissipation effect for extended "Coherence'', for example, Jos generation of Josephson neurons and synapses are practically possible via Josephson contacts with tunable critical current, hybrid superconductor ferromagnetic structures. Such tunable non-linear circuit elements with memory can be created [3].

The most dominating factor is experiments and direct work with new quantum nano-materials. But technical utilization and optimization for improved quantum nano-electronic devices need theoretical research methodology.

II. Characteristics of Modeling Nano structured Materials Using Non-QFT Quantum Mechanical Methods.

Here we will briefly discuss some important conventional quantum mechanical methods and related good approximation models for the structures and properties of nano materials [4]. We start with Schrodinger differential time dependent wave equations to explain atomic and electronic structure, dynamics and properties of nano systems. For the exact solution of it is simplified by adiabatic approximation or Born-Oppenheimer approximation [5] with Hamiltonian including spin state. Further simplified approach was given by Hartee-Fock approximation [6], considering electrons move in an average field gradually refined.

The following matrix determinant is obtained for multi-electron wave function as:

$$\Psi(\vec{r_1}, \vec{s_1} \ldots, \vec{r_{Ne}}, \vec{s_{Ne}}\, t) = \frac{1}{\sqrt{Ne!}} \det[\Psi_i(\vec{r_j}, \vec{s_j})] \ldots\ldots\ldots\ldots(1)$$

Where $\vec{r}$ = radius vectors; $\vec{s}$ = spin vectors; Ne = Total number of electrons.

The first in the Density Functional Theory (DFT) group is Thomas-Fermi Theory [7] with weakly interacting particles as almost all characteristics of nano system is determined by its electron density. Kohn- Sham [8] proposed more advanced approach by elaborating the Hohenberg-Kohnfunctional FHK as

$$F_{HK}\left[n\left(\vec{r}\right)\right] = T_S\left[n\left(\vec{r}\right)\right] + \frac{1}{2}\iint \frac{n(\vec{r})n(\vec{r'})}{|\vec{r'}-\vec{r}|} d\vec{r}\, d\vec{r'} + E_{XC}\left[n\left(\vec{r}\right)\right] \ldots\ldots\ldots\ldots(2)$$

Where, T_S=Kinetic energy; E_{XC} = Exchange co-relational contribution to energy.

The more accurate exchange correlation energy is given by Meta Generalized Gradient Approximation (MGGA) [7]. Further accurate quantum dynamical methods like Born-Oppenheimer Molecular Dynamics (BOMD)[8] or Car-Parrinello Molecular Dynamics (CPMD)-[9] are suitable for metals (conductors), semiconductors and di-electric nano system.

Some recent accurate approximation methods in this regard are Attached Plane Wave (APW), Atomic Sphere Approximation (ASA), Vannier Functions (VF), base selection in the form of Muffin Tin Orbitals (MTO), Gaussian Orbitals (GO), Slater Type Orbitals (STO) etc.

III. Theoretical Modeling of Nano structured Materials Using Quantum Field Theory (QFT) With Feynman Diagram

"Fictitious bodies" or "quasi particles" or "renormalized particles" and Collective Excitations (CE).

To find the characteristic properties of QP or CE i.e., "effective mass", "lifetime", probability "amplitude" and "energy" of them in the Many Body System (MBS), QFT (QED) introduces a physical parameter called "propagator" or "Greens function" which describes and links all type of interaction in the nano system with accuracy in a universal way like one particle propagator two particles (electron-hole)propagator, no particle propagator(vacuum amplitude) etc.[11].

Fig (1 and 2) below shows all the configuration of the particles and holes which maybe kicked up by the bare particles as it propagates through many bodies nano-system at particular time t0(dashed line). We can use GR as retarded Green's function propagator for electron and GA as advanced green function propagator for hole.

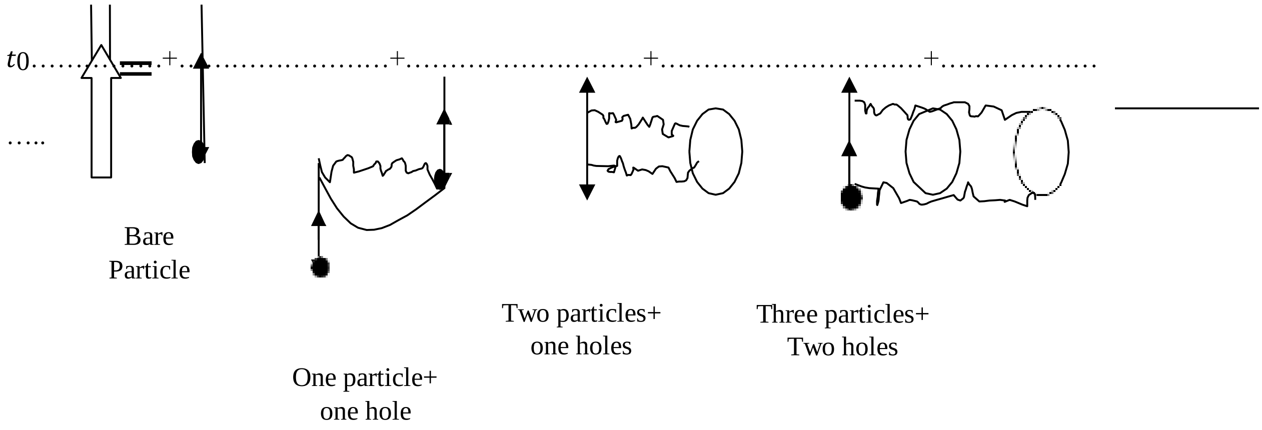


Fig-(1)

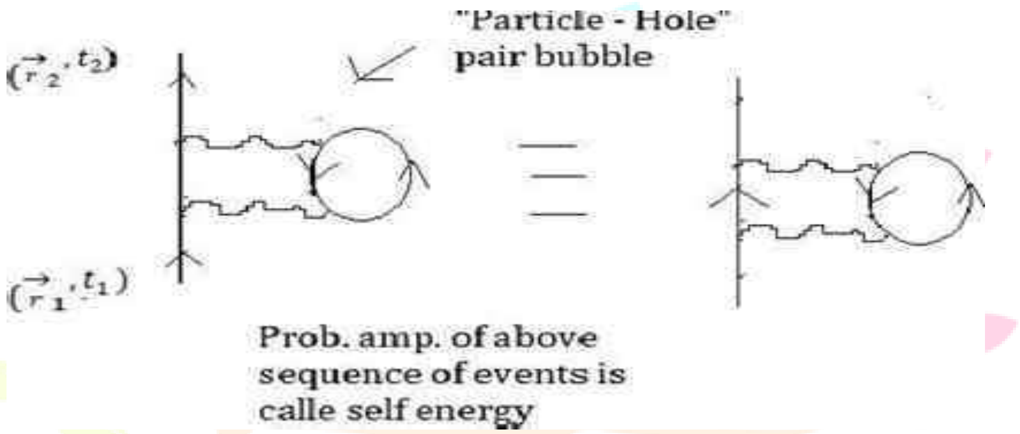


Fig-(2)

Now if we compare quasi-particle (QP) in Fig (1) then ever-changing cloud of particles and holes surrounding the bare particle (BP) has converted it into quasi-particle (QP).

Why do we need QFT? To explain it let us consider Dirac's relativistic quantum mechanical equation for electron (positron) as this approach utilizes Clifford (Geometric) algebra in complex vector (Hilbert) space, convenient in terms of QFT for a nano-system.[12].

Dirac's equation in Lorentz Covariant (Tensor) form in natural units (i.e.=c=1) as

$$\left(-i\gamma^{\mu}\frac{\partial}{\partial x^{\mu}} - m\right)\psi(x^{\mu}) = 0................(3)$$

Or in another equivalent form as:

$$\left(i\beta\frac{d}{dt} + \vec{\alpha}.\vec{\nabla} - m\right)\psi(t,\vec{x}) = 0.........................(4)$$

Where the terms have the usual meaning and α, β, γ are Dirac's Matrices.

The equation (4) can be thought of as kind of "square root" of Klein-Gordon equation which gives quantum dynamics of bosons (e.g.-photon) and follows Bose-Einstein quantum statistical mechanism like Fermi-Dirac Statistics restricted by Pauli 'exclusion principle. Therefore, in a relativistic theory, fluctuations of the vacuum energy (Casimir effect-experimentally verified) are to allow the creation of particle-antiparticle pair electron-positron out of the vacuum to be seen how the multi particle interpretation is forced upon us by relativistic invariance. Relativistic invariance forces the introduction of quantum field as when we insist in keeping a single particle interpretation that we crash against causality violations.

We consider Dirac four component spinors ψ (in 4D) as equivalent to two, two component Weyl right-handed chiral (helicity) and left-handed chiral spinors u+ and u- (in 2D) respectively for parity invariance theory.

The general solution to the Dirac's equation with $k^0 = \omega_k = \left(|\vec{k}|.|\vec{k}| + m^2\right)^{0.5}$, including creation and annihilation operators $\hat{b}^\dagger$ and $\hat{b}$ for particle (electron) respectively and $\hat{d}^\dagger$&$\hat{d}$ for antiparticle (positron) respectively with positive energy solution u and negetive energy solution v as

$$\hat{\psi}(t,\vec{x}) = \int \frac{d^3k}{(2\pi)^3 \times 2\omega_k} \sum_{s=\pm 1/2} \left[u(\vec{k},s)\hat{b}(\vec{k},s)e^{-i\omega_k.t+i\vec{k}.\vec{x}} + v(\vec{k},s)\hat{d}^\dagger(\vec{k},s)e^{i\omega_k.t-i\vec{k}.\vec{x}}\right] \text{................(5)}$$

With more accurate Hamiltonian: $\hat{H}$:by removing divergent contribution with the normal order prescription is

$$:\hat{H}: = \sum_{s=\pm 1/2} \int \frac{d^3k}{(2\pi)^3 \times 2\omega_k} \left[\omega_k \widehat{b_k} \ldots\ldots..\right] \qquad \text{................................(6)}$$

Indicating four vector gauge potential $(\phi,\vec{A})$ with Lorentz invariant gauge fixing condition $\partial\nu A\nu = 0$ $and \partial\nu F^{\mu\nu} = 0$, $satisfies$ Klein-Gordan quantum field equation for the boson (e.g., photon).

Lorentz invariant electrodynamics equation using four vector gauge potential $A\mu(\phi,\vec{A})$ and the anti-symmetric rank two field strength tensor $F\mu\nu$ indicating $A\mu$satisfies Klein-Gordan quantum field equation for the boson (e.g., photon), $A\mu$ can expanded in the complete basis of the solution of Dirac's spinor as

$$\widehat{A_\mu}(t,\vec{x}) = \sum_{\lambda=\pm 1} \int \frac{d^3k}{(2\pi)^3 \times 2|\vec{k}|} \left[\epsilon_\mu(\vec{k},\lambda)\hat{a}(\vec{k},\lambda)e^{-i|\vec{k}|.t+i\vec{k}.\vec{x}} + \epsilon_\mu(\vec{k},\lambda)\hat{a}^\dagger(\vec{k},\lambda)e^{-i|\vec{k}|.t+i\vec{k}.\vec{x}}\right] \qquad \text{.............(7)}$$

Where λ=±1represents the helicity (polarization) of photon and $\epsilon_\mu(\vec{k},\lambda)$as solution to the equation of motion. The Langrangian of spin (1/2) field coupled (interaction) to electro-magnetism is written as

$$\propto_{QED} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}(i\gamma^\mu D_\mu - m)\psi \text{ ....(8)}$$

Where the terms have the usual meaning.

By plugging in quantized covariant Maxwell field equations into the Langrangian we find that interaction between fermion and photon to be

$$\propto_{QED}{}^{(int)} = -eA_\mu\bar{\psi}\gamma^\mu\psi \quad \text{...........................(9)}$$

With current density four vector in Dirac's theory, $j^\mu = e\bar{\psi}\gamma^\mu\psi$.

QED is a form of QFT based on the Abelian gauge symmetry of local unitary U (1) phase rotation. This interaction part of the action S containing a relativistic "photon quantum field" and a "Spinor quantum field" and its Hermitian conjugate as

$$S_{QED} = \int d^4x\,[-\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}(i\gamma^\mu D_\mu - m)\psi eA_\mu\bar{\psi}\gamma^\mu\psi] \text{...................(10)}$$

is shown in Feynman's diagram Fig-(3), the vertex V.

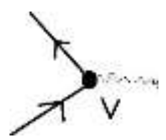


Fig- (3) FD of interaction part of Poincare invariant action S

Using Feynman rules, corresponding amplitude for contribution of each corresponding one can be calculated. The basic concept is, each of its building blocks from the given diagram (vertices and external, internal lines) with associated contribution from the corresponding diagram can be computed. As shown in fig. (4), the following correspondence for vertices and internal propagators for QED in the Feynman gauge. The extra piece in the photon propagator is indicated by a change in gauge.

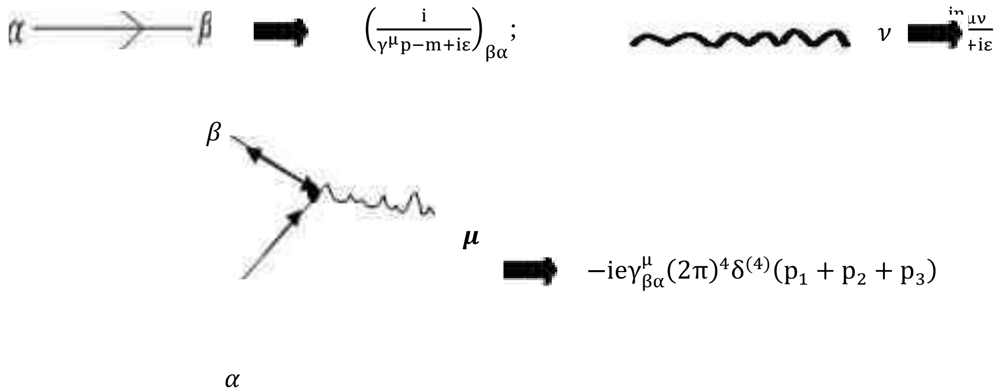


Fig- (4) FD of building blocks with propagators for QED

For renormalization of the charge to eliminate in finite terms the partial sum for QED which takes into account first correction of the propagator of the virtual photon, exchanged due to vacuum polarization as shown in Fig-(4) with Corresponding expression where the diagram between brackets is given by Fig- (5) With corresponding expression for the interaction Hamiltonian.

$$H_{int} = e\int d^4 x A_{\mu}\overline{\psi}\gamma^{\mu}\psi \qquad \ldots\ldots\ldots(11)$$

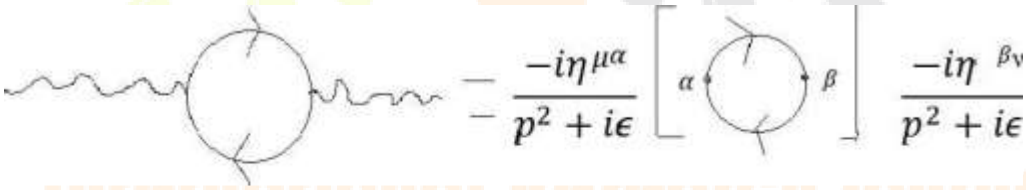
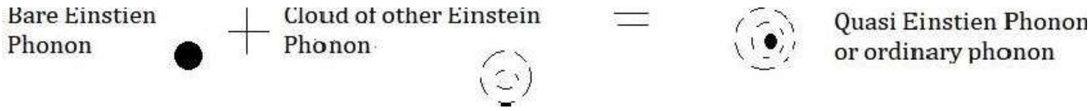


Fig-(5) FD with expression for propagator expansion

By implementing gauge invariance and using standard techniques in the Computation of Feynman diagrams [13,14], the polarization tensor $\prod\mu\nu$(q) defined in Fig-(5) the bracketed part can be written as (Setting scale dependent renormalization with me=0)

$$\prod(q)=(q^2\eta\mu\nu-q\mu q\nu)\prod(q^2) \qquad \ldots\ldots (12)$$

Where the momentum q is the total momentum of the virtual electron- position pair by propagating photon in the intermediate channel.



Fig– (6) Formation of quasi-Einstein phonon

In a nano-crystal system with quantum lattice oscillations (phonon) as MBS can be expressed as the sum of (i) an unperturbed part describing a very primitive sort of collective excitation (CE) called "Einstein phonon" and (ii) a perturbation describing the interactions among "Einstein phonon" quantum field. On accounting the interaction, the Einstein phonon becomes surrounded by a cloud of other Einstein phonons; this dress it and converts it into an ordinary phonon as shown in Fig-(6). Hence the ordinary phonon can be interpreted as a quasi-particle (QP) in quasi collective excitations (CE), Similar to quasi-Plasmon.

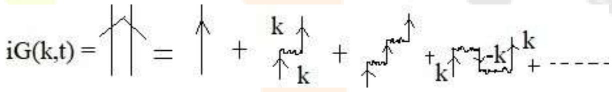
The renormalized Einstein phonon frequencies i.e. well-known phonon dispersion law is generated by calculating summation of self-energy diagrams (Feynman) accurately to all orders with the pole of the resultant clothed propagator. By setting the quasi-particle (QP) or collective excitations (CE) with the phonon, field theoretic path (QED or QFT) is utilized.[5].

The Bosonic operators $\hat{a}_k^{\dagger}$ and $\hat{a}_k$, yields Hamiltonian H as

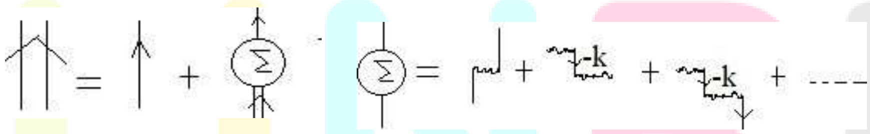
$$H = \sum_k \omega_k \left(\hat{a}_k^{\dagger} \cdot \hat{a}_k + \frac{1}{2}\right) \ldots\ldots\ldots\ldots\ldots\ldots (13)$$

With dispersion law, $\omega = \omega_0\sqrt{(1 - \cos kd)}$ and ground state energy, $E = \sum_k \frac{\omega_k}{2}$.

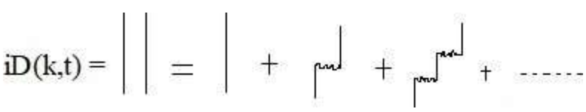
Now using Dyson's perturbating equation for evaluation of phonon propagator as shown in Fig-(7)



(a) Expansion of Einstein phonon propagator



(b)Dyson Equation (c) Irreducible Self energy expansion



(d)Expansion of Einstein phonon propagator

Fig– (7)

Fig-(7) yields in (k,ω) space (Fourier transformed) with free propagator D_0 as

$$iD\,(k,\omega) = iD_0[1+(iD_0)(-iv_k+i(iD_0)^2(-iv_k)^2+\ldots\ldots]=\frac{iD_0}{1-D_0V_k} \quad \ldots\ldots(14)$$

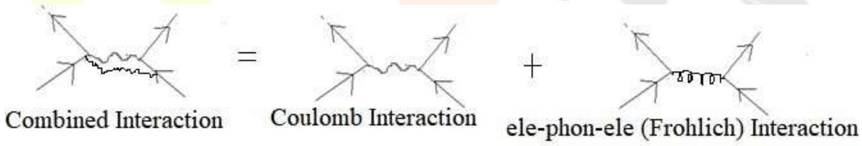
With iD_0 for each line and $-iv_k$ for each wiggle, gives

$$D\,(k,\omega)=\frac{2\omega_0}{\omega^2-\omega_0{}^2[1-\cos kd]}\simeq\frac{2\omega_0}{\omega^2-\omega_k{}^2+2i\delta\omega_k} \quad \ldots\ldots(15)$$

And the final result

$$E = E_0 + \sum \text{linked graphs} = \sum_{k>0} \omega_0[1-\cos kd] = \sum_k \frac{\omega_k}{2} \quad \ldots\ldots(16)$$

In more complex nano-solid superconducting crystal system, then the net Hamiltonian is given by {with reference to FD in Fig-(8)}as



Fig– (8) FD of interaction mechanism in superconducting nano-crystal.

$$H_{tranf}=H_{quasi-electron}+H_{sheilded-coulomb}+H_{ele-phon-ele}+H_{dressedphonon}+ \ldots\ldots(17)$$

Where$H_{quasi-electron}=\sum_{k,}{}^{\dagger}{}_{k,\,\sigma}C_{k,\sigma}$;$H_{dressedphonon}=\sum_k\hbar\omega_k\left(\bar{B}_k{}^{\dagger}\bar{B}_k+\frac{1}{2}\right)$.

Now, it is defined systematically a set of observable critical exponents, exponents of scaling laws that describe quantum thermodynamic effect in the vicinity of the critical point. It can be shown, using Callan-Symanzik equation that all these exponents can be reduced to two basic an anomalous dimension [15].

The above facts can be utilized for a comparative test with these important predictions of QFT to experimental results away from the critical points, two-point correlation function G (x) should decay exponentially according to (<s(x)>≠0)

$$G(x)\sim e^{-|x|} \quad \ldots\ldots(18)$$

With G(x)=<s(x)s(0)>; s(x)=spin field.

We expect correlation length ξ should increase to infinity in terms of exponent as

$\xi \sim |t|^{-\nu}$ ……………………………………………………………………(19)

The parameter t can point out to characteristic approach to critical point as

$t=\frac{T-T_C}{T_C}$ …………(20)

With T=any temperature; T_C= critical temperature.

Power law decay is set for correlation function exactly at t=0. G(x)can be expressed in terms of exponent η by the formula

$G(x) \sim \frac{1}{|x|^{d-2+\eta}}$ ……….(21)

Where d is the Euclidian space dimension.

The Langrangian strongly moves towards fixed points of the renormalization group in the field of long-range correlation. In d<4, this is the Wilson-Fisher fixed points. Ind≥4, it is the free field fixed points.

The specific heat capacity C_H of the quantum thermodynamic nano-system at fixed external magnetic field, H =0 in terms of exponent α as

$C_H \sim |t|^{-\alpha}$……………………………………………………………………(22)

Ordering sets in at t=0, the magnetization M at H=0 as $t \rightarrow 0$ from below, M in terms of another exponents β *and* δ as

$M \sim |t|^{\beta}$ and $M \sim H^{\delta}$ ……………………………………………………………(23)

Finally, the magnetic susceptibility χ diverges at critical point, the divergence is in terms of exponent γ as

$X \sim |t|^{-\gamma}$……………………………………………………………………(24)

Equations (18-24) define a set of critical exponents' $\alpha, \beta, \gamma, \delta, \nu, \eta$ which can be measured experimentally for a variety of quantum thermodynamical nano-systems.

The following tabular data (Table-1) gives the comparative theoretical value of critical exponents for both QFT and non-QFT quantum mechanical framework and experimental values for statistical quantum nano-system [16].

Table-1

Critical Exponent		Non-QFT QM Methods	QFT Framework	Experimental result	Statistical Nano systems
	γ	1.230	1.241	1.240	Binary Liquid
	ν	0.632	0.630	0.625	Binary Liquid
N=1 System	α	0.103	0.110	0.113	Binary Liquid
	β	0.329	0.325	0.325	Binary Liquid
	η	0.032	0.020	0.016	Binary Liquid
	γ	1.320	1.316	1.315	Super Fluid He^4
N=2 System	ν	0.674	0.670	0.672	Super Fluid He^4
	α	0.010	-0.007	-0.013	Super Fluid He^4
	γ	1.386	1.401	1.400	EuO,EuS(Ferromagnetic)
	ν	0.711	0.705	0.700	RbNn$F3$(Antiferromagnetic)
N=3 System	α	-0.111	-0.090	-0.011	EuO,EuS, RbNn$F3$
	β	0.365	0.371	0.370	EuO,EuS
	η	0.041	0.033	0.035	EuO,EuS

Where N= Number of fluctuating spin components/quantum thermodynamic variable components at the critical point.

IV. Practical Applications of Nanostructured Materials for Quantum Electronic Devices

There are wide range of applications for functional nanostructured materials in all types of energy efficient and cost-effective electronic devices including quantum electronic devices (spinotronics) [11].

We start with the estimate of effective mass of quasi-electron $m^* = \frac{\hbar^2}{\frac{\partial^2 E}{\partial k^2}} = 0.13 m_e, m_e$ = electronic rest mass

$= 9.1 \times 10^{-31}$ kg for CdSe/ZnS nano materials QD (quantum dot) material (Zero-dimensional nano-material) from

QFT or other QM theoretical prediction. For heterostructure or composite nano materials, effective mass is a tensor of rank two as $m_{ij}^* = \frac{\hbar^2}{\frac{\partial^2 E}{\partial k_i \partial k_j}}$.

"QDLED" Light Emitting Diodes) of all color range with nano-materials In P, ZnSe, ZnS, GaN, $CsPb(Br)_3$, $CsPbI_3$, CdSe, CdS, SiO_2, PbS, Graphene oxide etc. QD solar cell with nanomaterial Si, ZnO, TiO_2, Nb_2O_5 etc utilized for non-conventional energy resources in remote areas and hybrid vehicles. Single electron (SE) quantum electronic devices like SE box, SET (transistor /oscillators) in the regime of "Coulomb Blockade" with nano-materials Al, AlO_X, CdSe, Ti, Si, SiO_2 etc.

CNT (Carbon Nano Tube) a one-dimensional nano material and graphene sheet (2D material) for FET (Field Effect transistor) in modern nano-electronic devices. In Micro-Electro-Mechanical-Systems (MEMS) and Nano-Electro-Mechanical systems (NEMS) with nano materials Si, Au, Ni, Al, SiC, Ag, Polymer etc. In modern day applications of QD (0D) or QR(1D) or QS (2D) nano materials also include medical imaging devices as in HDCT, CTMRI and in quantum computers, SQUID (Super Conducting Quantum Interference Devices) etc.

V. Conclusion

We can design quantum nano-materials depending on the type of applications using QFT based analysis. QFT and other good quantum mechanical methods undoubtedly occupy a key position in the study of "nano systems" characteristic properties. Various modifications and assumptions are able to eliminate limitation of the quantum theoretical methods as well as reduce complexity and dimensionality of solved problems by reducing the number of investigated object's degrees of freedom.

As for example in calculating vacuum amplitude using QED (QFT) we took "flat space time" for relativistic quantum fields or is to be replaced by "curved space time"

We need to apply more accurately to explore "quasi-particle–poisoning-protected topological quantum computation with Majorana "Zero modes" using QFT with FD. In July 2021 a case of formation of "quantum time crystal" state (sixth state of matter) or 4D quantum material in the quantum processor of Google's" SYCAMORE "20 qubits quantum computers were reported to exist. It is a future research possibility to model such systems using QFT with FD for efficiency enhancement.

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