The 'Generalized Skettrup Model' and Matsubara statistics

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The 'Generalized Skettrup Model' (GSM) [1] links features of near-band gap and intra-gap *electronic* as well as corresponding *optical* spectra of polycrystalline and spatially non-homogeneous amorphous semiconductors and insulators to probabilities of *fluctuations* in an energy of the individual quasi-particle, number of quasi-particle in a quantum grand canonical ensemble (QGCE) of *confined acoustic phonons* with plane-wave basis, and their aggregate energy. Features of the GSM are discussed herein in comparison to those of quantum statistics pioneered by Japanese physicist T. Matsubara [2], which takes into account fluctuations in *temperature* of QGCE. The GSM [1] might be ultimately treated as a 'conservative' **counterpart** of the generic Matsubara statistics for the specific case of ensemble of acoustic phonons confined within micrometer- and sub-micrometer-sized non-homogeneities (grains) of polycrystalline and spatially non-homogeneous amorphous semiconductors and insulators. However, scope of the GSM might be expanded further based on the fundamental idea, pioneered by T. Matsubara.

1. Introduction

The Generalized Skettrup Model (GSM) depicted in the *second* chapter of ref. [1] (see also references therein) is essentially based on evaluation of probabilities of *fluctuations* in an *energy* of individual acoustic phonon, their *aggregate energy* and (generally rational) *number* of quasi-particles of the (quantum) *grand canonical* ensemble (QGCE) corresponding to many-particle *bosonic* (phononic) excitations in amorphous and/or crystalline solids. In particular, within the GSM framework, those fluctuation probabilities are customarily evaluated via an *integration* (averaging) over available (at the given aggregate energy of the ensemble) quantum states of acoustic phonons and appropriate number of those quasi-particles, which yield the given aggregate energy of the ensemble [1]. Furthermore, the GSM implies that those fluctuations in the ensemble of *confined* longitudinal (acoustic) phonons are linked intimately to energy fluctuations in an *electronic* sub-system of a semiconductor (insulator) and eventually to its corresponding optical spectra: relationship between the *instantaneous* aggregate energies (fluctuation probabilities) of electronic and phononic sub-systems might be established quantitatively either based on semi-empirical electron-phonon coupling parameters or via the 'deformation potential' formalism [1].

Aforementioned GSM approach essentially implies that individual and aggregate *energies* as well as *number* of quasi-particles in the phononic ensemble have to be treated as *real* (generally rational) *variables*, while temperature of the ensemble is usually treated as a *fixed* (constant) quantity for the given environmental conditions (i.e., as a *parameter* of an external 'thermal reservoir').

In contrast, quantum statistical mechanics pioneered (in particular) by famous Japanese physicist **Takeo Matsubara** for a quantum many-body system [2] treats the *temperature* of the QGCE (comprises either electrons (fermions) or phonons (bosons)) as a *variable complex parameter*, implying that the *temperature* of the ensemble *fluctuates* as well – *in addition* to fluctuations in total number of its quasi-particles as well as in their individual and aggregate energies for the given QGCE. Such treatment becomes essential for *interacting* systems: *condensed* matter, dense plasmas, neutron stars etc., where local temperature *fluctuations* are expected to be significant or dominant. Herein consequences of such effects are evaluated only for *solid* polycrystalline and amorphous semiconductors and insulators, including nano-structured ones, and discussed in comparison with features of the GSM [1].

2. Key Features of Matsubara statistics

The averaged (statistical) characteristics of many-body state(s) of a condensed (either fermionic or bosonic) ensemble at the given (absolute) temperature T might be evaluated based on the quantum grand canonical density operator, ρ_D [3]:

$$\rho_D \equiv \frac{\exp\left(-H_0 / k_B T\right)}{Tr\left[\exp\left(-H_0 / k_B T\right)\right]}, \qquad (1)$$

where $Tr[\exp(-H_0/k_B T)]$ denotes *trace* (i.e., sum of its *diagonal* elements) of the matrix exponential of the weighted 'thermal' Hamiltonian matrix $(H_0/k_B T)$, and k_B is the Boltzmann constant. This ρ_D operator is Hermitian, positive definite and normalized: $Tr\{\rho_D\} \equiv 1$ [3].

In an *equilibrium* state, the Hamiltonian H_0 of the system is expected to be constant (*time-independent*), and evolution (fluctuations) of the system characteristics have to be attributed entirely to the *fluctuation(s) in its local temperature*. Nevertheless, Eq.(1) remains valid even for *Heisenberg representation* of the quantum mechanics, which presumes that *wavefunctions* (set of basic states) of the system are *time-independent*, while the *operators* (Hamiltonian) do *change in time*.

In order to implement aforementioned many-body formalism to bosonic or fermionic ensembles, it is worth to note that the following generic identity holds [2, 3]:

$$\exp\left(-\beta H_0\right) \quad \equiv \quad \exp\left[-i\int\limits_0^{-i\beta} H_0(t)dt\right] \quad = \quad \exp\left[-\int\limits_0^\beta H_0(\Im)d\Im\right], \qquad (2)$$

where $i = \sqrt{-1}$, $\beta = 1/(k_B T)$, and $\Im = \beta/i$. Thus, it becomes possible to treat the $\exp(-H_0/k_B T)$ term as an *'evolution' operator* on the *imaginary time* scale $\Im$, as long as integration in Eq.(2) is fulfilled along the straight line, parallel to imaginary time on the complex time plane [2 – 4]. Indeed, in a very generic case, the *unitary* 'evolution' operator $U(t_0, t)$ satisfies a time-dependent Schrödinger's equation with the solution, which might be expressed in the form very similar to that of Eq.(2) [3]. Therefore, Eq.(2) might be eventually re-formulated in a more compact (and yet generic) form [3]:

$$U\left(t_0 - i\beta, t_0\right) \quad \equiv \quad \exp\left(-\beta \hat{H}_0\right). \qquad (3)$$

Again, due to Eq.(3), when the $\hat{H}_0$ Hamiltonian corresponds to an *equilibrium* state of a system (i.e. at $\hat{H}_0 = H_0$), the $U(t_0 - i\beta, t_0)$ operator might (formally) be identified as an evolution operator in *imaginary* time $\Im = \beta/i$, which propagates the system from its state at the initial time t_0 parallel to the imaginary time axis $t_0 - i\beta$ [2, 3]. Therefore, the (averaged) effect of fluctuations in the local temperature T of the (bosonic or fermionic) ensemble on its statistical characteristics might be taken into account via appropriate *integration* over the 'imaginary time' $\Im$ of the ensemble; such integration also yields a sort of '*interaction representation*' for the statistical ensemble [2 – 4]. It is noteworthy, that evolution of the bosonic ensemble is *periodic* on the imaginary time scale, while evolution of the fermionic ensemble is 'antiperiodic' [2 – 4]. Nevertheless, fluctuations (and 'interactions') in either phononic or fermionic ensemble might be taken into account via appropriate integration over the *imaginary* time scale of the given ensemble. The original Matsubara's idea is *tremendously fruitful* and was further developed and implemented for decades in quantum statistic of condensed matters: in particular, in so-called (equilibrium and non-equilibrium) 'Green's Function' (GF) formalisms of those systems [3, 4]. In addition, it was advanced further by T. Matsubara in order to set up *diagrammatic* perturbation theory for grand partition function within framework of the field-theoretical basis [2 – 4]. However, 'orthodox' GF and diagrammatic formalisms *do not apply* to '…Bose systems below points of the Bose condensation…' and '…Fermi systems in which superconductivity exists…' [4].

3. 'Matsubara correction' for GSM equations

The basic feature of the briefly depicted in the previous section Matsubara's generalization of the fluctuation concept might be incorporated *naturally* into the GSM framework. Indeed, basic equation of (isotropic version) of the GSM comprises the Gibbs's (exponential) term, number of available states of the QGCE of (confined) *acoustic* phonons as well as its 'partition function', Z_M [1]:

$$W_D(E_T) \quad \cong \quad \exp\left(-\frac{E_T}{k_B T}\right) \int\limits_{M0}^{M_M} \frac{1}{\Gamma(M+1)\left(Z_M\right)^{r2}} \left[\frac{2\,L_x\,L_y\,F(L_x,\,L_y,\,L_z)\,E_T^2}{M^{\,r1}\,(hc_s)^2}\right]^M dM\,, \qquad (4)$$

where $W_D(E_T)$ denotes probability density of finding of the ensemble of confined (within a crystallite, column, cone, etc.) acoustic phonons in a state with its aggregate energy of E_T, $\Gamma(M)$ is Euler's Gamma-

function [5], h is the Planck's constant, c_s is *longitudinal* sound velocity, L_x, L_y, L_z are length of the (orthogonal) ribs of parallelepiped phonon confinement volume, while dimensionless function $F(L_x, L_y, L_z)$ depends solely on *ratios* of the L_x, L_y and L_z parameters; see also Eq.(26a) in ref. [1]. Integration in Eq.(4) is expected to be fulfilled over the appropriate range of (generally rational) number M of acoustic phonons in the ensemble (this integration range is restricted by the M_M and $M0$ limits), while the (rational) model parameters $r1$ and $r2$ are typically varying in the following ranges: $0.5 \leq r1 \leq 2$; $0.5 \leq r2 \leq 1$ [1].

Formally, the *scalar* E_T quantity in the exponential term of Eq.(4) might be treated as particular case of a (single-valued) *equilibrium* Hamiltonian, which causes the system evolution only on the imaginary time scale $\Im$. Therefore, for this specific Hamiltonian, and based on Eq.(2), we have to evaluate the following 'evolution' exponential 'Matsubara' integral:

$$\Theta_M \left(E_T, T \right) \;=\; \exp\left[-i \int_0^{-i\beta} E_T \, d\Im \right], \quad (5)$$

where $\Im$ denotes imaginary time variable, while the *dimensionless* $\Theta_M(E_T, T)$ function (integral) depends both on the T and E_T quantities. Thus, Eq.(4) might be modified as follows:

$$W_D(E_T) \;\cong\; \Theta_M \left(E_T, T \right) \exp\left(-\frac{E_T}{k_B T} \right) \int_{M0}^{M_M} \frac{1}{\Gamma(M+1)\left(Z_M \right)^{r2}} \left[\frac{2 L_x L_y F(L_x, L_y, L_z) E_T^2}{M^{r1} (hc_s)^2} \right]^M dM . \quad (6)$$

As it was mentioned above, for bosonic (phononic) ensembles, boundary conditions have to be *periodic* on the imaginary time scale [2 – 4], see also Fig.1(a). Noteworthy, that left-hand half of the complex plane in this figure corresponds to *negative* Re[exp(iβE_T)] quantities, which directly implies *negative probability* [$W_D(E_T)$ function(s)] defined by the Eqs.(4, 6).

In order to overcome this problem, total contribution from 'Matsubara correction(s)' (expressed by the $\Theta_M(E_T, T)$ term in Eq.(6)), might be evaluated as well (following refs. [2, 3] and Eq.(5) herein) via summation over *Matsubara frequencies* ω_n – poles of the integrand in Eq.(5), Fig.1(b). Those frequencies are routinely defined for *bosonic* ensemble based on *periodicity* condition of the exponential term, Fig. 1(a). In particular: $\exp(i\beta\omega_n) \equiv 1$ [5]; $\Rightarrow \beta\omega_n = 2\pi n$ or $\omega_n = 2\pi k_B T n$ (n herein is an integer index) [2, 3]. At $T = 1$ K and $n = 1$, this periodicity condition yields: $\omega_1 = 2\pi k_B T \cong 5.414 {\ast} 10^{-4}$ eV. The higher Matsubara frequencies are just proportional (topple) to the ω_1 quantity, Fig. 1(b).
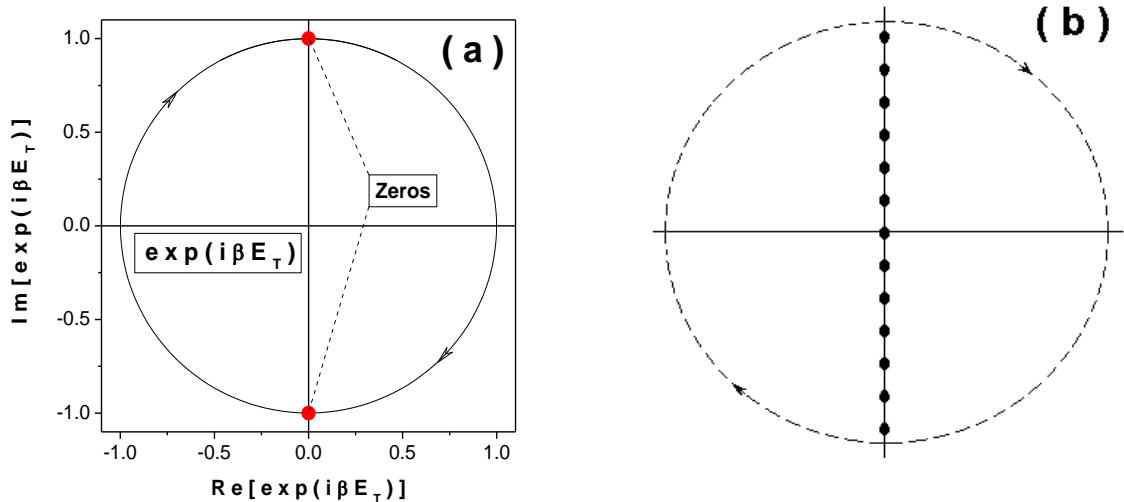

FIG.1 (a), (b) (color online). Schematic illustration of (**a**) periodic behavior of the *inverse* exponential term in Eq.(4) on the complex plane, with two its zeros located on the imaginary axis, and (**b**) the Matsubara integration contour (solid lines and dashed curves). The black dots in figure (**b**) are located on the *imaginary* (time) axis indicate positions of the *bosonic* Matsubara frequencies. See also figure (**a**) and main text for more details.

Conventionally, summation over mentioned above Matsubara frequencies might be replaced with *integration* over contour defined in the *complex time plane*, and stretched over the imaginary time range from $-i\beta$ to $i\beta$ [2, 3] (see also Fig.1(b)). It is noteworthy, that $\beta = 1/k_BT \cong 11605$ eV^{-1} at T = 1 K, while its *dimensionless* counterpart $\underline{\beta} = E_T/k_BT \cong 11605$ at $E_T = 1$ eV. This implies that the integration contour in Fig. 1(b) would contain $\Theta_M(E_T, T) = 2\underline{\beta} = E_T/(\pi k_BT) \cong 3.694_*10^3$ of the *equally separated* (see Fig. 1(b)) poles, and this number actually defines the dimensionless 'Matsubara correction' factor $\Theta_M(E_T, T)$ to the exponential term in Eq.(6) at T = 1 K and $E_T = 1$ eV. Furthermore, the correction factor $\Theta_M(E_T, T)$ is apparently *strongly affected* both by the temperature T of the 'reservoir' and E_T quantity: it is *directly proportional* to E_T at the *fixed* T but *inversely proportional* to T at the *fixed* E_T. Therefore, the 'Matsubara correction' factor becomes just of $\Theta_M(E_T, T) \cong 3.69$ at T = 1000 K and $E_T = 1$ eV – i.e., three orders of the magnitude *smaller* than the 'low-temperature' one at the same E_T quantity. Temperature and spectral behavior(s) of the dimensionless $\Theta_M(E_T, T)$ function are also illustrated in Figs.2.(a), (b), respectively.
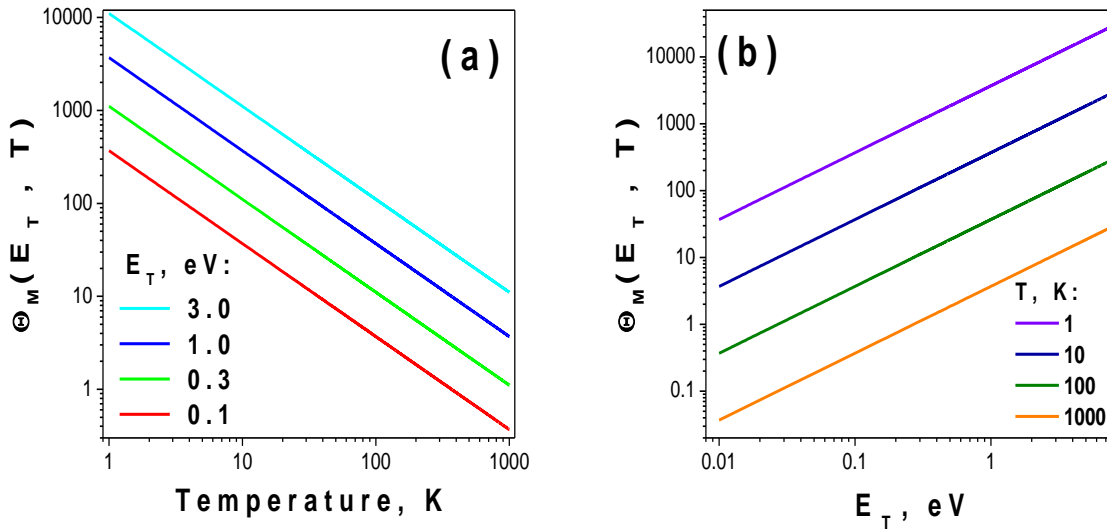

FIG. 2(a), (b) (color online). Effects of (**a**) the absolute temperature T and (**b**) aggregate energy E_T of the phonon ensemble on the $\Theta_M(E_T, T)$ function. Mind double-logarithmic scale(s) for both panels of the figure.

Based on results, discussed above in the main text, and illustrated in Fig. 2(b), the *dimensionless* 'Matsubara correction' term $\Theta_M(E_T, T)$ apparently might be represented as a *linear function* of E_T at a given temperature T:

$$\Theta_M\left(E_T, T\right) = \Theta_M^0\left(E_{\min}, T\right) * E_T, \qquad (7)$$

where $E_{\min}$ is a low limit of aggregate energy of the ensemble of acoustic phonons, imposed by presence of morphology (non-homogeneities) in the studied (isotropic but spatially non-homogeneous) polycrystalline or amorphous semiconductor (insulator), and defined by the Eq.(18B) in ref. [1], while $\Theta_M^0(E_{\min}, T) = [\Theta_M(E_{\min}, T)/E_{\min}]$ is a *dimensional* (of eV^{-1}) and *temperature-dependent* factor; Eq.(7) valids at $E_T \geq E_{\min}$. Therefore, based on Eq.(15D) in ref. [1], the 'partition function', Z_M, for the 'isotropic version' of the Eq.(6) reads:

$$Z_M = \theta_M^0\left(E_{\min}, T\right) \left(k_BT\right)^{[2(M+1)]} \Gamma\left[\left(2M+2\right), \left(\frac{E_{\min}}{k_BT}\right), \left(M\frac{k_B\theta_D}{k_BT}\right)\right] \left[\frac{2L_x L_y F(L_x, L_y, L_z)}{M^{r1}(hc_s)^2}\right]^M, \qquad (8)$$

where $\Gamma(m, z_0, z_1)$ is the 'generalized incomplete Gamma function' [5] with m = (2M + 2), $z_0 = (E_{\min}/k_BT)$, $z_1 = [M * k_B\theta_D/(k_BT)] = M\theta_D/T$. It is noteworthy that the *dimension* of Z_M functions defined

by Eq.(8) is still expressed in eVs; i.e., it remains *unchanged* as compared to its counterpart expressed by Eq.(15D) in ref. [1]: enlargement in the (rational) power of the (k_BT) term is 'compensated' by appearance of the dimensional $\Theta^0_M(E_{min}, T)$ one. Thus, though the dimensionless 'Matsubara correction' function $\Theta_M(E_T, T)$ well exceeds 10^3 at T ≈ 1 K and $E_T > 1$ eV (Fig. 2(b)), its ultimate effect on the $W_D(E_T)$ distribution defined by the Eq.(6) would be eventually reduced due to 'normalizing' effect of the partition function Z_M (statistical sum). This 'Matsubara correction' might be also embedded naturally into an *anisotropic* version of the GSM [1].

Thus, the depicted above 'Matsubara correction' is expected to work well for *crystalline* and (probably) even *liquid* semiconductors and insulators at a *finite* temperature. Furthermore, the 'Matsubara correction' is expected to *remain valid* even at *zero* temperature for many *amorphous* solid semiconductors and insulators, where spatial atomic positions are commonly expected to be fixed – though generally *affected* by the 'freeze-in' temperature established at the material formation (see Eq.(37) on p.81 of ref. [1]). In other words, those atomic positions are still subjected to evolution in the 'imaginary time', though 'traditional' meaning of the 'imaginary time' has to be amended, and rather linked to the (inverse) *'freeze-in'* temperature – than to actual absolute temperature of the material. It is noteworthy, that different versions of the *GSM* enable such kind of 'Matsubara correction(s)' readily, while many others well-known approaches to simulation of intra-gap electronic density-of-states (DOS) in disordered semiconductors (e.g., the semi-classical [6] and Halperin-Lax [7] ones) do not comprise the exponential 'Gibbs' term and might not be 'corrected' in this way. Furthermore, in spite of certain *formal* similarity among the path-integral-based formalism [8] and Matsubara one, the physical backgrounds of those formalism and even their mathematical expressions are essentially different. Indeed, the *real-time action* (i.e. a time-dependent integral over a potential) in the canonical path integral formalism has to be transformed into *imaginary-time* integration within framework of Matsubara's approach via (formal) implementation of so-called 'Wick rotation', see ref. [9], p.12. In general, both path-integral and Matsubara formalisms are equally applicable to bosonic and fermionic ensembles, though the path-integral usually *oscillates far more strongly* (with alterations in its sign!) as its argument enlarges, mainly due to relatively low $\hbar$ quantity (the *dimensional* $k_BT/\hbar$ ratio is ~1.309 x 10^{11} at T = 1 K in appropriate SI units). Therefore, the path-integral technique was usually implemented (e.g., refs. [8, 10, 11]) to relatively small (with the typical spatial extent of just very few Angstroms) parts of *electronic* sub-system, *interacting* with their atomic (phononic) counterparts, while direct contributions from the quantized atomic vibrations (phonons) are usually 'integrated out' (eliminated) within the path-integral cum Lagrangian formalisms [8, 10, 11].

The overall contribution even from non-normalized 'Matsubara correction' to the basic equations of the GSM is expected to be relatively *small* for *polycrystalline* and *spatially non-homogeneous amorphous semiconductors and insulators* with the typical sizes of non-homogeneities (grains) of the order of **~ 1 μm** – or even sub-micrometer – (especially at elevated – e.g. room – temperature T and relatively low ($E_T < 1$ eV) aggregate energy of the phonon ensemble) as compared to effects caused by variation in the GSM model parameters r1 and r2 in Eqs.(4, 6). Indeed, contribution from the main integrand term in Eqs.(4, 6) (located within square bracket in those equations) is ~2.400×10^9 at $E_T = 1$ eV, M = 1, r2 = 2 and r2 = 1 for the <100>–oriented polycrystalline *diamond* with $L_x = L_y = L_z = 1$ μm, and *exceeds* even low-temperature contribution from $\Theta_M(E_T, T)$ term by a factor of ~6.50×10^5. Similar differences are expected as well for others polycrystalline and spatially non-homogeneous amorphous semiconductors and insulators, when dimensions L_x, L_y and L_z of their non-homogeneities are of $L_x \approx L_y \approx L_z \approx 1$ μm. The statement on relatively *insignificant* room-temperature 'Matsubara corrections' for ensemble of acoustic phonons confined within grains, columns, cones (etc.) of those *polycrystalline* and *spatially non-homogeneous amorphous semiconductors and insulators* at *elevated temperatures* might be verified independently: integration over the imaginary time is expected to yield just a *partition function* (for the aforementioned bosonic ensemble) at β → 0 (i.e., at T → ∞) limit(s), see details on p.13 of the ref. [9].

On the other hand, both aforementioned contribution might be *well comparable* for **nano-structured** semiconductors and insulators (e.g., when $L_x \approx L_y \approx L_z \approx 10$ nm) at low temperature and relatively high aggregate energy: contribution from the integrand term in Eqs.(4, 6, 8) is expected to be reduced by ~6 orders of the magnitude (as compared to the discussed above case of the <100>-oriented polycrystalline diamond), while contribution from the 'Matsubara correction' function $\Theta_M(E_T, T)$ remains unaffected by alterations in the sizes of the non-homogeneities. In other words, the 'Matsubara correction' becomes *well comparable* with the mentioned above integrand term and becomes really *important* for *nano-structured* semiconductors and insulators only: the $\Theta_M(E_T, T)$ term might dominate their behavior at low absolute temperature T and relatively high aggregate energy of the ensemble E_T.

4. Conclusions

In summary, the GSM presented in ref. [1] might be treated as a kind of 'conservative' **counterpart** to the well-known quantum Matsubara statistics (and closely related to it equilibrium (Matsubara) and non-equilibrium GF formalisms [2 – 4]) for the aforementioned particular cases of ensemble(s) of acoustic phonons confined within polycrystalline and spatially non-homogeneous amorphous semiconductors and insulators with micrometer- and sub-micrometer sizes of non-homogeneities (grains), though the GSM apparently is not applicable directly to the ensemble of the fermions and essentially uses the Debye's *plane wavefunctions basis*, while other convenient sets of basis functions (e.g., eigenfunctions of the quantum harmonic oscillator, QHO) might be used as well in the GF formalism(s) [2, 3]. On the other hand, the plane wave-functions basis of acoustic phonons implemented within the GSM framework [1] allows one to use effectively advantages of the phononic *DOS concept*, *simplify considerably* final equation(s) of the GSM, *incorporate it naturally* into conventional framework(s) of the *solid state* and *statistical physics*, as well as takes into account <u>long-range</u> (e.g., *coherent*, *morphological*) and <u>anisotropic effects</u> (if any) in polycrystalline and spatially non-homogeneous amorphous semiconductors and insulators [1], while routine implementation of others sets of the basic functions (e.g., QHO eigenfunctions) might not allow to utilize aforementioned advantages [3], and apparently would yield in (much) more time- and resource-demanding calculations.

It is essentially, that following the fundamental idea pioneered by T. Matsubara [2], basic equations (of different versions) of the GSM might be 'corrected' in order to take into account effects of fluctuations in the absolute and/or 'freeze-in' temperature(s) of the ensemble of the confined acoustic phonons (via implementation of the dimensionless $\Theta_M(E_T, T)$ function, as it discussed in the previous section), though such corrections are expected to be almost negligible for polycrystalline and spatially non-homogeneous amorphous semiconductors and insulators with micrometer- and sub-micrometer sizes of non-homogeneities (grains), but might be significant or even dominant for their nano-structured counterparts. In addition, the model parameters r1 and r2 of the GSM, are typically invariable (fixed) for the given set of simulations even though the T and E_T quantities may vary in this set [1], while the introduced above $\Theta_M(E_T, T)$ function is clearly temperature- and energy- dependent, see Figs.2.(a), (b). This distinction inspires further development of the GSM, and its direct implementation to the nano-structured semiconductors and insulators. For such a case, the model parameters r1 and r2 of the GSM might be re-defined readily as the energy- and temperature-dependent ones, following the 'Matsubara style'.

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