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Statistical Mechanics Involving Fractal Temperature

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Abstract: In this paper, the Schrödinger equation involving a fractal time derivative is solved and corresponding eigenvalues and eigenfunctions are given. A partition function for fractal eigenvalues is defined. For generalizing thermodynamics, fractal temperature is considered, and adapted equations are defined. As an application, we present fractal Dulong-Petit, Debye, and Einstein solid models and corresponding fractal heat capacity. Furthermore, the density of states for fractal spaces with fractional dimension is obtained. Graphs and examples are given to show details.

Keywords: local fractal calculus; middle- τ Cantor sets; fractal Einstein solid models; fractal Debye solid models; fractal heat capacity

1. Introduction

Fractal geometry explains fractal shapes with self-similarity, scale invariance, and fractional dimensions, which have found many applications in science and engineering [1–4]. Analysis on fractals has been studied by different methods such as harmonic analysis, stochastic processes, fractional spaces, and calculus [5–20].

A fractal model was used to perform analysis of averaged micromotions in mesoscale and complex systems and considered as a path for curing cancers [21–23]. The mechanisms of tumor growth and angiogenesis were investigated by considering their fractal structure [22,23].

Scale relativity is a generalization of relativity theory to the concept of scale, using fractal geometries to get scale transformations. Einstein claimed that space-time is curved, Nottale said that space-time is curved and fractal, which means that space-time is a non-differentiable manifold [24–26]. The Schrödinger equation was solved on a Sierpinski gasket involving a well potential using the finite element method [27]. Fractional path integration was considered as an action on fractals to find the ground state energy for a fractionally perturbed oscillator [28].

A Riemann-like calculus which is called fractal calculus was formulated on fractal sets, which is algorithmic and simple for application [29–33]. Fractal calculus was applied in optics to find diffraction patterns of fractal gratings and mean square displacement of random walks on fractal sets [34–36]. Stochastic Langevin equations were studied which give fractal mean square displacements of under-damped, over-damped, and ultra-slow fractal scaled Brownian motions. The annual mean surface air temperatures in Hungary had fractals structure with a mean fractal dimension of 1.23 ± 0.01 [37]. Harmonic analysis has been used to solve Schrödinger equation on the fractal Sierpinski gasket and to find energy spectrum [38–43]. Fluid was mixed inside by using the fractal structure [33].

Continuing in the vein of the research mentioned above, we generalize thermodynamics with fractal temperature and the corresponding statistical mechanics and solid-state physics models.

The outline of our paper is the following. In Section 2, we give a brief summary of fractal calculus. In Section 3, we solve the Schrödinger on thin Cantor sets and obtain the corresponding eigenvalues or energy spectrum. In Section 4, we present thermodynamics and statistical mechanics involving fractal temperature and physical models which might be useful for fitting experimental data. Section 5

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provides density of states for a physical system with fractional-dimension spaces. Section 6 is devoted to our conclusion.

2. Basic Tools

We present the steps which yields to middle- ω Cantor set or thin Cantor-like set. The thin Cantor-like sets have Lebesgue measure zero and fractional Hausdorff dimension [44].

The middle- ω Cantor set or thin Cantor-like set is generated by following steps:

(1) Take an open interval of length $0 < \omega < 1$ from the middle of the J = [0, 1], namely

$$C_1^{\omega} = [0, \frac{1}{2}(1-\omega)] \cup [\frac{1}{2}(1+\omega), 1].$$
 (1)

(2) Cut and take disjoint open intervals of length ω from the middle of the remaining closed intervals of step 1, namely

$$C_2^{\omega} = \left[0, \frac{1}{4}(1-\omega)^2\right] \cup \left[\frac{1}{4}(1-\omega^2), \frac{1}{2}(1-\omega)\right] \cup \left[\frac{1}{2}(1+\omega), \frac{1}{2}((1+\omega) + \frac{1}{2}(1-\omega)^2)\right] \cup \left[\frac{1}{2}(1+\omega)(1+\frac{1}{2}(1-\omega)), 1\right].$$
(2)

:

(m) Remove disjoint open intervals of length ω from the middle of the remaining closed intervals of step m-1.

$$C^{\omega} = \bigcap_{m=1}^{\infty} C_m^{\omega}.$$
 (3)

The Hausdorff dimension of C^{ω} is given by

$$\dim_{H}(C^{\omega}) = \frac{\log 2}{\log 2 - \log(1 - \omega)},\tag{4}$$

where $H(C^{\omega})$ is the Hausdorff measure which was used to derive Hausdorff dimension [44].

Local Fractal Calculus

The flag function of $C^{\omega} \subset J = [b_1, b_2]$ is defined by [29–31],

$$\mathbf{F}(C^{\omega}, \mathbf{J}) = \begin{cases} 1, & \text{if } C^{\omega} \cap \mathbf{J} \neq \emptyset, \\ 0, & \text{otherwise.} \end{cases}$$
 (5)

Then, $P^{\alpha}[C^{\omega}, W]$ is defined by [29–31] by

$$P^{\alpha}[C^{\omega}, W] = \sum_{i=1}^{m} \Gamma(\alpha + 1)(t_i - t_{i-1})^{\alpha} \mathbf{F}(C^{\omega}, [t_{i-1}, t_i]).$$
 (6)

where $0 < \alpha \le 1$, $\Gamma(.)$ is gamma function, and $W_{[b_1,b_2]} = \{b_1 = t_0, t_1, t_2, \dots, t_m = b_2\}$ is a subdivisions of J.

The **mass function M** $^{\alpha}(C^{\omega}, b_1, b_2)$ is defined in [29–31] by

$$\mathbf{M}^{\alpha}(C^{\omega}, b_{1}, b_{2}) = \lim_{\delta \to 0} \left(\inf_{\mathbf{W}_{[b_{1}, b_{2}]} : |\mathbf{W}| \leq \delta} \mathsf{P}^{\alpha}[C^{\omega}, \mathbf{W}] \right)$$
$$= \lim_{\delta \to 0} \mathbf{M}^{\alpha}_{\delta}, \tag{7}$$

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where, infimum is taking over all subdivisions W of $[b_1, b_2]$ satisfying $|W| := \max_{1 \le i \le m} (t_i - t_{i-1}) \le \delta$. The **integral staircase function** $S_{C^{\omega}}^{\alpha}(t)$ is defined in [29,30] by

$$S_{C^{\omega}}^{\alpha}(t) = \begin{cases} \mathbf{M}^{\alpha}(C^{\omega}, b_0, t), & \text{if} \quad t \ge b_0, \\ -\mathbf{M}^{\alpha}(C^{\omega}, b_0, t), & \text{otherwise,} \end{cases}$$
(8)

where b_0 is an arbitrary and fixed real number.

The γ -dimension of a set $C^{\omega} \cap [b_1, b_2]$ is defined

$$\dim_{\gamma}(C^{\omega} \cap [b_1, b_2]) = \inf\{\alpha : \mathbf{M}^{\alpha}(C^{\omega}, b_1, b_2) = 0\}$$
$$= \sup\{\alpha : \mathbf{M}^{\alpha}(C^{\omega}, b_1, b_2) = \infty\}. \tag{9}$$

Remark 1. For the any compact fractal sets $\alpha = \dim_{\gamma}(C^{\omega}) = \dim_{H}(C^{\omega})$ [29,30].

The C^{α} -limit of a function $\mathbf{g}: C^{\omega} \to \Re$ at $t \in C^{\omega}$ is given by

$$\forall \epsilon > 0, \ \exists \delta > 0 \text{ such that for any } z \in C^{\omega} \text{ and } |z - t| < \delta \Rightarrow |\mathbf{g}(z) - \ell| < \epsilon.$$
 (10)

If ℓ exists, then we denote

$$\ell = C_{-}^{\alpha} \lim_{z \to t} \mathbf{g}(z). \tag{11}$$

Examples of a thin Cantor-like set, staircase function, Characteristic function and the γ -dimension of thin Cantor-like set in the particular case $\omega = 1/3$ are graphed on Figure 1.

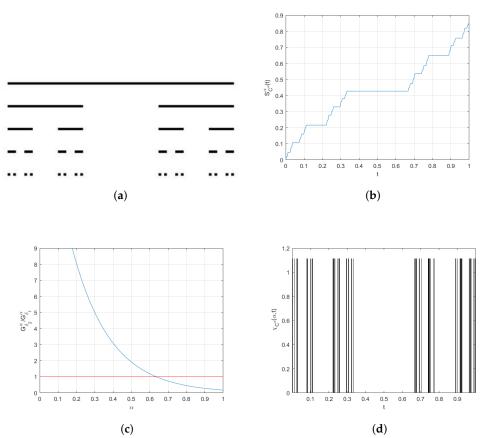


Figure 1. Figures for the Section 2. (a) Thin Cantor-like set with $\omega = 1/3$; (b) Staircase function corresponding to thin Cantor-like set with $\omega = 1/3$; (c) The γ -dimension of thin Cantor-like set with $\omega = 1/3$; (d) Characteristic function for Cantor-like set with $\omega = 1/3$.

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The function $\mathbf{g}: C^{\omega} \to \Re$ is C^{α} -continuity if for any point $t \in C^{\omega}$ the equality

$$\mathbf{g}(t) = C_{-}^{\alpha} \lim_{z \to t} \mathbf{g}(z),\tag{12}$$

holds.

The C^{α} -derivative of $\mathbf{g}(t)$ at t is defined by [29]

$$D_{C^{\omega}}^{\alpha}\mathbf{g}(t) = \begin{cases} C_{-}^{\alpha} \lim_{z \to t} \frac{\mathbf{g}(z) - \mathbf{g}(t)}{S_{C^{\omega}}^{\alpha}(z) - S_{C^{\omega}}^{\alpha}(t)}, & \text{if } t \in C^{\omega}, \\ 0, & \text{otherwise,} \end{cases}$$
(13)

if the limit exists.

The C^{α} -integral of $\mathbf{g}(t)$ on $J = [b_1, b_2]$ is defined in [29–31] and approximately given by

$$\int_{b_1}^{b_2} \mathbf{g}(t) d_{C^{\omega}}^{\alpha} t \approx \sum_{i=1}^{n} \mathbf{g}(t_i) (S_{C^{\omega}}^{\alpha}(t_i) - S_{C^{\omega}}^{\alpha}(t_{i-1})).$$
 (14)

For more details we refer the reader to [29,30].

The Characteristic function of the middle- ω Cantor set is defined in [31] by

$$\chi_{C^{\omega}}(\alpha,t) = \begin{cases} \frac{1}{\Gamma(\alpha+1)}, & t \in C^{\omega}, \\ 0, & otherwise. \end{cases}$$
 (15)

Subsequently, we intend to give our main results.

3. Shrödinger Equation on Thin Cantor Sets

The Shrödinger equation in quantum mechanics provide wave function and energy levels for the physical system [45–50]. In this section, we consider Schrödinger equation on fractal $C^{\omega} \times \Re$ as follows

$$\frac{-\hbar^2}{2m}(D_x^{\alpha})^2\psi^{\alpha}(x,t) + v(x)\psi^{\alpha}(x,t) = i\hbar\frac{\partial\psi^{\alpha}(x,t)}{\partial t}, \quad x \in C^{\omega},$$
(16)

where

$$v(x) = \begin{cases} 0, & 0 \le x \le 1, \\ \infty, & elsewhere, \end{cases}$$
 (17)

with boundary conditions

$$\psi^{\alpha}(0,t) = \psi^{\alpha}(1,t) = 0. \tag{18}$$

The v(x) in Equation (17), represent the infinite-well potential. By conjugacy of ordinary and fractal calculus [29,30], the solution of Equation (16) is given by

$$\psi^{\alpha}(x,t) = \sum_{n=1}^{\infty} e^{-iE_n^{\alpha}t/\hbar} \varphi_n^{\alpha}(x), \tag{19}$$

where

$$E_n^{\alpha} = \frac{\pi^2 \hbar^2 n^2}{2m S_{C\omega}^{\alpha}(1)}$$

$$= \frac{\pi^2 \hbar^2 n^2}{2m \Gamma(\alpha + 1)}, \quad n = 1, 2, ...,$$
(20)

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where E_n^{α} is called fractal energy spectrum, m is the mass of a particle, and \hbar is the Planck constant [45–47]. The fractal eigenfunction of Hamiltonian or the solution of time-independent Shrödinger equation is as follows [45–47]:

$$\varphi_n^{\alpha}(x) = \sqrt{\frac{2}{S_{C^{\omega}}^{\alpha}(1)}} \sin\left(\frac{\pi n S_{C^{\omega}}^{\alpha}(x)}{S_{C^{\omega}}^{\alpha}(1)}\right)$$

$$= \sqrt{\frac{2}{\Gamma(\alpha+1)}} \sin\left(\frac{\pi n S_{C^{\omega}}^{\alpha}(x)}{\Gamma(\alpha+1)}\right). \tag{21}$$

In Figure 2, we have sketched Equation (21) for the cases of $\alpha=1$, 0.63 and n=1, 2. Since $0 \le S_{C\omega}^{\alpha}(x) \le x^{\alpha}$, then we can write

$$\varphi_n^{\alpha}(x) \approx \sqrt{\frac{2}{\Gamma(\alpha+1)}} \sin\left(\frac{\pi n x^{\alpha}}{\Gamma(\alpha+1)}\right).$$
(22)

In Figure 3, we have plotted eigenvalues (E_n^{α}) for the case of the different dimensions (Figure 3a), and the upper bound of the fractal wave functions; that is Equation (22) which associate with the eigenvalues (Figure 3b).

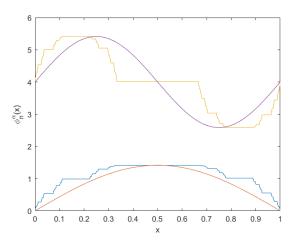


Figure 2. Graph of $\varphi_n^{\alpha}(x)$ setting n = 1, 2, and $\alpha = 1$, 0.63.

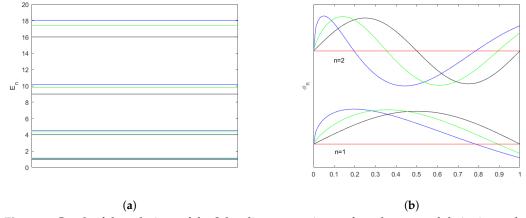


Figure 3. Graph of the solutions of the Schrödinger equation on fractal space and their eigenvalues. (a) Energy levels verses by space dimension, $\alpha = 1$ (black), $\alpha = 0.5$ (blue), $\alpha = 0.75$ (green); (b) Upper bound of the fractal wave function corresponding to space dimension, $\alpha = 1$ (black), $\alpha = 0.5$ (blue), $\alpha = 0.75$ (green).

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4. Partition Function on Thin Cantor-Like Sets

In this section, we suggest a generalized thermodynamics framework base on fractal space and temperature. The analogue of canonical ensemble partition function on the fractals sets is denoted by $z^{\alpha,\mu}$ and defined by [51,52].

$$z^{\alpha,\mu} = \sum_{n=1} \exp\left(-\frac{E_n^{\alpha}}{k_B S_{C^{\omega}}^{\mu}(T)}\right),\tag{23}$$

where k_B is Boltzmann constant and μ is the fractal dimension of temperature ($T \in C^{\mu}$). The analogue of the probability of every microstate n on fractal set is defined by

$$P_n = \frac{1}{z^{\alpha,\mu}} \exp\left(-\frac{E_n^{\alpha}}{k_B S_{C^{\omega}}^{\mu}(T)}\right). \tag{24}$$

In view of conjugacy of ordinary and fractal calculus, energies of system N particles in fractal space are given by

$$E^{\alpha,\mu} = Nk_B S_{C\omega}^{\mu}(T)^2 D_T^{\mu} \ln z^{\alpha,\mu}$$

$$\approx Nk_B T^{2\mu} D_T^{\mu} \ln z^{\alpha,\mu}.$$
(25)

The important point to note here is that by setting $\mu = 1$ we can get standard result [51,52]. The fractal heat capacity is defined by

$$C^{\alpha,\mu} = D_T^{\mu} E^{\alpha,\mu}. \tag{26}$$

The fractal Boltzmann's entropy is defined by

$$\mathcal{M}^{\alpha,\mu} = Nk_B \ln z^{\alpha,\mu} + Nk_B S^{\mu}_{C\omega}(T) D^{\mu}_T \ln z^{\alpha,\mu}. \tag{27}$$

The fractal Helmholtz free energy denoted by, $H^{\alpha,\mu} = E^{\alpha,\mu} - T\mathcal{M}^{\alpha,\mu}$, is defined by

$$H^{\alpha,\mu} = -Nk_B \ln z^{\alpha,\mu}. \tag{28}$$

Example 1. Let consider energy of a paramagnetic material as follows:

$$E^{\alpha,\mu} = -NB\nu_B \tanh\left(\frac{\nu_B B}{k_B S_{C^{\omega}}^{\mu}(T)}\right),\tag{29}$$

where v_B is Bohr magneton. Then using Equation (26), we have

$$C^{\alpha,\mu} = Nk_B \left(\frac{2\nu_B B}{k_B S_{C^{\omega}}^{\mu}(T)}\right)^2 \frac{\exp(-\frac{E_n^{\mu}}{k_B S_{C^{\omega}}^{\mu}(T)})}{\left(1 + \exp(\frac{2\nu_B B}{k_B S_{C^{\omega}}^{\mu}(T)})\right)^2}.$$
 (30)

We now apply $S^{\mu}_{C^{\omega}}(T) < T^{\mu}$, to obtain

$$C^{\alpha,\mu} \approx Nk_B \left(\frac{2\nu_B B}{k_B T^{\mu}}\right)^2 \frac{\exp(\frac{2\nu_B B}{k_B T^{\mu}})}{\left(1 + \exp(\frac{2\nu_B B}{k_B T^{\mu}})\right)^2}.$$
 (31)

In Figure 4 we have sketched the fractal heat capacity of paramagnetic materials versus dimensions.

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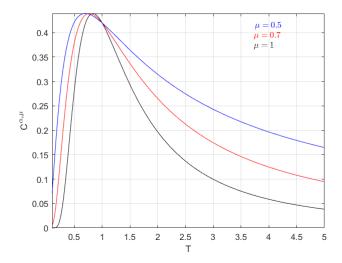


Figure 4. Graph shows the fractal heat capacity of paramagnetic materials respect to dimension of fractal temperature.

Example 2. Suppose a system with two energy levels as the following

$$E_0 = 0 E_1 = \frac{\pi^2 \hbar^2}{2m\Gamma(\alpha + 1)}.$$
 (32)

The partition function of the system is

$$z^{\alpha,\mu} = 1 + \exp\left(-\frac{\pi^2 \hbar^2}{2mk_B \Gamma(\alpha + 1)S_{C^{\omega}}^{\mu}(T)}\right). \tag{33}$$

It follows that

$$E^{\alpha,\mu} = \frac{\frac{k_B a}{\Gamma(\alpha+1)}}{1 + \exp\left(-\frac{a}{\Gamma(\alpha+1)S_{C\omega}^{\mu}(T)}\right)} \exp\left(-\frac{a}{\Gamma(\alpha+1)S_{C\omega}^{\mu}(T)}\right),\tag{34}$$

where

$$a = \frac{\pi^2 \hbar^2}{2mk_B}. (35)$$

Using Equation (26) we have

$$C^{\alpha,\mu} = \frac{k_B a^2}{\Gamma(\alpha+1)^2 S_{C^{\omega}}^{\mu}(T)^2} \frac{1}{\left(1 + \exp(-\frac{a}{\Gamma(\alpha+1)S_{C^{\omega}}^{\mu}(T)})\right)^2} \exp\left(-\frac{a}{\Gamma(\alpha+1)S_{C^{\omega}}^{\mu}(T)}\right).$$
(36)

Using upper bound $S^{\mu}_{C^{\omega}}(T) \leq T^{\mu}$ we have

$$C^{\alpha,\mu} \approx \frac{k_B a^2}{\Gamma(\alpha+1)^2 T^{2\mu}} \frac{1}{\left(1 + \exp(-\frac{a}{\Gamma(\alpha+1)T^{\mu}})\right)^2} \exp\left(-\frac{a}{\Gamma(\alpha+1)T^{\mu}}\right). \tag{37}$$

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Example 3. The fractal analogue of energy system for the **Einstein solid-state model** is given by

$$E^{\alpha,\mu} = \frac{3N\mathcal{E}}{\exp\left(\frac{\mathcal{E}}{k_B S_{C\omega}^{\mu}(T)}\right) - 1},$$
(38)

where $\mathcal{E} = h\nu$, is the energy of photon, $h = 2\pi\hbar$, and ν is the frequency of light. Then by Equation (26) we obtain

$$C^{\alpha,\mu} = \frac{3N\mathcal{E}^2}{k_B S_{C^{\omega}}^{\mu}(T)^2} \frac{\exp\left(\frac{\mathcal{E}}{k_B S_{C^{\omega}}^{\mu}(T)}\right)}{\left[\exp\left(\frac{\mathcal{E}}{k_B S_{C^{\omega}}^{\mu}(T)}\right) - 1\right]^2}.$$
(39)

Using upper bound $S^{\mu}_{C^{\omega}}(T) \leq T^{\mu}$ we get

$$C^{\mu} = \frac{3N\mathcal{E}^2}{k_B T^{2\mu}} \frac{\exp\left(\frac{\mathcal{E}}{k_B T^{\mu}}\right)}{\left[\exp\left(\frac{\mathcal{E}}{k_B T^{\mu}}\right) - 1\right]^2}.$$
 (40)

In Figure 5, we present fractal heat capacity for a solid by considering fractal Einstein model setting different dimensions.

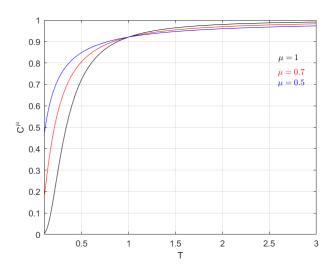


Figure 5. Graph shows Einstein solid model for case of fractal temperature with different dimensions.

Example 4. The energy of system of particles in the **Dulong–Petit solid model** on the fractal temperature is given by

$$E^{\alpha,\mu} = 3Nk_B S^{\mu}_{C^{\omega}}(T). \tag{41}$$

Then the fractal heat capacity of the system will be

$$C^{\mu} = 3Nk_B \frac{1}{\Gamma(1+\mu)}.\tag{42}$$

The fractal analogous to the energy of a system in the Debye solid-state model is given by

$$E^{\alpha,\mu} = \frac{3Nk_B \pi^4 S_{C^{\omega}}^{\mu}(T)^4}{5\theta_D^3}.$$
 (43)

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An easy computation gives

$$C^{\mu} = \frac{12}{5} \pi^4 N k_B \left(\frac{S^{\mu}_{C^{\omega}}(T)}{\theta_D} \right)^3, \tag{44}$$

where θ_D is constant and called Debye temperature. Then we have

$$C^{\mu} = \frac{12}{5} \pi^4 N k_B \frac{T^{3\mu}}{\theta_D^3}.$$
 (45)

In Figure 6, we have plotted Equation (45) for the different values of μ .

Remark 2. Please note that the Einstein and the Debye solid model are valid to low temperature limit.

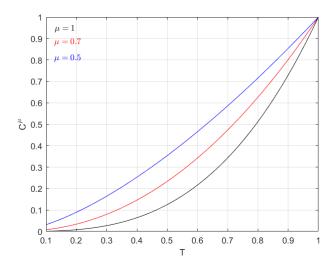


Figure 6. Graph preset Debye solid model for the fractal temperature with different dimensions.

5. Density of States in Fractal Spaces

The density of states (DOS) have important role in solid-state physics which is denoted by g(E) and its valve for a 0-, 1-, 2- and 3-dimensional systems are given in the following [49–51]

$$g(E) \propto \delta(E),$$
 0 – dimension,
 $g(E) \propto E^{-1/2},$ 1 – dimension,
 $g(E) \propto constant,$ 2 – dimension,
 $g(E) \propto E^{1/2},$ 3 – dimension. (46)

Now, the DOS for the fractal system is suggested by

$$g(E) \propto E^{-\alpha_1/2}, \qquad 0 < \alpha_1 < 1,$$

 $g(E) \propto E^{\alpha_2/2}, \qquad 1 < \alpha_2 < 3,$ (47)

where $\alpha_2 \neq 2$.

In Figure 7 we have plotted DOS for the systems with different dimensions.

Remark 3. In this paper, upper indices μ and α stand for fractal dimension but ω indicate the ratio of [0,1] we have removed for building fractal thin Cantor-like sets.

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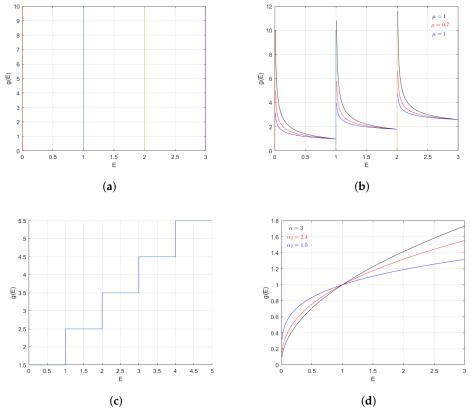


Figure 7. DOS for the systems with fractional and integer dimensions. (a) DOS for the system with dimension 0; (b) DOS for the system with dimensions 1, 0.7 and 0.5; (c) DOS for the system with dimension 0; (d) DOS for the system with dimensions 3, 2.4 and 1.5.

6. Conclusions

In this paper, we have given a generalization of thermodynamics which includes fractal derivatives. For applications of suggested mathematical models, the heat capacity for permanganic materials and systems with two energy levels have been derived. Fractal Dulong-Petit, Debye and Einstein solid models have been studied to include the model for wider material which might have a fractal structure. Finally, the DOS for fractals with fractional dimension has been suggested to provide a new mathematical model in solid-state physics.

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