Phase transition in the bounded one-dimensional multitrap system

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Abstract

We have previously discussed the diffusion limited problem of the bounded one-dimensional multitrap system where no external field is present and pay special attention to the transmission of the diffusing particles through the imperfect traps. We discuss here the case in which an external field is included to each trap and find not only the transmission but also the energy associated with the diffusing particles in the presence and absence of such a field. From the energy we find the specific heat $C_h$ and show that for certain values of the parameters associated with the multitrap system it behaves in a manner which is suggestive of phase transition. Moreover, this phase transition is demonstrated not only through the conventional single peak at which the specific heat function is undifferentiable but also through the less frequent phenomenon of double peaks.

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I. INTRODUCTION

The diffusion of classical particles in the presence of traps have been studied by various authors \([1, 2, 3, 4, 5]\). The idea of imperfect traps was introduced in \([6]\) and elaborated further by others \([7, 8]\) which study, especially, the nearest neighbours distance in the presence of a single imperfect trap. We note that the imperfect trap may represent a model for many real physical situations that are not easy to tackle directly. Among these one may enumerate all the reactions, including the chemical ones, in which the results for the reacting particles can not be predicted beforehand. That is, these reactions may result in either the elimination of some of the reacting particles or changing the values of some physical parameters that are associated with them. Among these parameters one may mention, for example, the transmission and absorption coefficients of the diffusing particles, their energy and the other variables derived from it such as the specific heat, the entropy etc. In \([9, 10]\) the transmission properties of these particles in the presence of \(N\) imperfect traps, without any external field, were intensively discussed for both cases of large and small \(N\). It was found \([9]\) that the larger is \(N\) the higher is the transmission so that for \(N \to \infty\) the probability that all the particles diffuse through all the traps tends to unity.

In this work we include an external field to each trap and find the effect of it upon the diffusing particles. We note that the case of a bias field in the presence of a single imperfect trap at the origin was discussed by Condat \textit{et al} in \([8]\) which studied among other things the effect of a uniform field on the distribution of nearest neighbours distances. In this work we introduce the bounded multitrap system and discuss not only the transmission that results from including an external field to each trap but also the energy associated with the diffusing particles. This energy is discussed for both cases of the existence and absence of a field and we show that it is highly sensitive to the presence of it so that increasing its intensity by a small amount may result in a disproportionally large change in the energies of the diffusing particles.

We note that although the physical situation is not strictly of the equilibrium kind we follow the tendency of many authors \([11]\) to discuss phase transition and specific heat even at situations which are far from equilibrium. In this context we note that it is well known that diffusion on a lattice can be mapped onto an equilibrium polymer problem \([12]\). Note that the imperfect traps, which introduces the diffusivity in the multitrap system, are characterized
here by a rather small constant trapping rate (denoted by $k$) as may be seen from the numerical work in which we assume $k = 1$ compared to the value of $k = \infty$ for the ideal traps. Thus, the bounded multitrap array deviates only slightly from equilibrium. Also, the fields added to this equations are entirely uniform as realized from the numerical part of this work. We may, therefore, discuss the specific heat and other thermodynamical variables.

We show in the following that the mentioned large changes in the energy entail, for certain values of the parameters associated with the multitrap system, corresponding large and even discontinuous changes in the specific heat $C_h$ derived from it. That is, the specific heat actually goes through phase transition which is demonstrated not only through the conventional undifferentiable single peak but also through double peaks [13, 14, 15, 16, 17, 18, 19]. We note that double peak phase transitions were found [14] in the analogous quantum one-dimensional bounded multibarrier potential. Lieung and Neda [15] and also Kim et al [16] have found double peaks in the form of the responsive curves which are apparently associated with dynamically induced phase transitions. Tanaka et al [17] have found such double peaks in antiferromagnetic materials corresponding to magnetic phases where the external magnetic field has a corresponding role to the parameter $c$ here. Ko and Asakawa [19] have found also double peaks with regards to the phases of the quark-gluon plasma which may be thought of as a large number of interactions in a bounded region.

In Section 2 we represent the appropriate terminology and terms associated with the one-dimensional bounded imperfect multitrap system as in [9, 10]. We then show, using the $N(2X2)$ transfer matrices method [20, 21], that for certain values of the parameters associated with the multitrap system the transmission probability through all the traps tends to unity in the presence of an external field. This was shown [9, 10], for the absence of field, by applying the same method. Using the results of Section 2 we calculate in Section 3 the energy associated with the diffusing particles for both cases of the presence and absence of a bias field. For this we use the single $(4NX4N)$ transfer matrix (as done in [9]) for calculating the coefficients of the density of the diffusing particles. In Section 4 we calculate the relevant specific heat $C_h$ and show that for certain values of the variables associated with the bounded system it behaves in a manner which is suggestive of phase transition. This is demonstrated in the presence of an undifferentiable discontinuous peaks in the curves of $C_h$ as function of the temperature. Moreover, as noted, we find for some values of the relevant variables that this phase transition is demonstrated in the form of double peaks. We then
calculate the relevant critical exponents associated with these phase transitions. In Section 5 we conclude with a brief summary.

II. THE ONE-DIMENSIONAL BOUNDED IMPERFECT MULTITRAP SYSTEM

We assume that the imperfect traps, through which the particles diffuse, are all characterized by the same width that depends upon their number \(N\) and the length \(L\) of the system.

That is, denoting the total width of the \(N\) traps by \(a\) and the total interval among them by \(b\) we can see that the width of each is \(\frac{b}{N}\) and the interval between any two neighbours is \(\frac{b}{N}\). We define as in [9, 10] the ratio \(c = \frac{b}{a}\) and express \(a\) and \(b\) in terms of \(c\) and the total length \(L = a + b\) as \(a = \frac{L}{1 + c}\), \(b = L \frac{c}{1 + c}\). The one-dimensional imperfect multibarrier system is assumed to be arrayed along the positive \(x\) axis so that it begins from the point \(x = \frac{b}{N} = \frac{Lc}{N(1+c)}\) and ends at \(x = L\). We also assume that at \(t = 0\) the particles are concentrated, except for an initial configuration \(f\), at the left hand faces of the \(N\) traps. The locations of these faces, according to the mentioned arrangement of the multitrap system, is given by

\[
\hat{x}_m = m \frac{Lc}{N(1+c)} + (m - 1) \frac{L}{N(1+c)}, \quad 1 \leq m \leq N \tag{1}
\]

It is assumed that each trap have the same field associated with it so that any particle that approach it may be, depending on the direction of the field, either attracted or repelled by it. The corresponding initial and boundary value problem associated with the one-dimensional bounded imperfect \(N\) trap system is [8, 9, 10]

\[
\rho_t(x, \hat{x}_m, t) = D \rho_{xx}(x, \hat{x}_m, t) - V \rho_x(x, \hat{x}_m, t), \quad 0 \leq x, \hat{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0
\]

\[
\rho(x, \hat{x}_m, 0) = e^{-\frac{V \hat{x}_m}{2D}} \delta(x - \hat{x}_m) + f(x, \hat{x}_m, 0), \quad 0 \leq x, \hat{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0 \tag{2}
\]

\[
\frac{\partial \rho}{\partial x}
|_{x=\hat{x}_m} = (k + \frac{V}{D}) \rho(\hat{x}_m, t), \quad 0 \leq \hat{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0,
\]

where \(\hat{x}_m\) denotes the left hand face of the \(m\)-th trap (see Eq (1)). \(\rho(x, \hat{x}_m, t)\) is the density of the diffusing particles and \(D\) is the diffusion constant which is considered to have two values; \(D_i\) inside the traps and \(D_o\) outside them [9, 10]. We note that one may generally find in the literature values of \(D\) in the range \(0.9 \geq D \geq 0.3\) (see, for example, p. 337 in
where it is noted that $0.5 \frac{m^2}{sec}$ is the order of magnitude of $D$ at room temperature and atmospheric pressure). We have assigned here for $D_o$ and $D_i$ the respective values of 0.8 and 0.4. $\rho_t(x, \dot{x}_m, t)$ and $\rho_{xx}(x, \dot{x}_m, t)$ are respectively the first time derivative and the second spatial derivative. The parameter $V$ is the diffusion velocity that results from the presence of the field and its magnitude and sign represent respectively the intensity and direction of the field. The second equation of the set (2) is the initial condition at $t = 0$ the first term of it signifies, through the $\delta$, that there is an initial concentration of the particles at the left hand face of the trap located at $x = \dot{x}_m, \ 1 \leq m \leq N$. The second term at the right hand side denotes an additional initial configuration of the density that depends upon $x$ and $\dot{x}_m$. The third equation is the boundary value condition which introduces the velocity $V$ that results from the field. The parameter $k$ denotes the degree of imperfection of the traps (in it is termed the trapping rate) so that in the limit $k \rightarrow \infty$ the trap becomes ideal in which case any particle that approaches it is absorbed. We follow the procedure in [9, 10] for $V = 0$ and decompose the set (2) into two secondary sets as follows

$$\rho_t(x, \dot{x}_m, t) = D\rho_{xx}(x, \dot{x}_m, t) - V\rho_x(x, \dot{x}_m, t), \quad 0 \leq x, \dot{x}_m \leq L,$$

$$1 \leq m \leq N, \quad t > 0,$$

$$\rho(x, \dot{x}_m, 0) = e^{-\frac{V\dot{x}_m}{2D}}\delta(x - \dot{x}_m), \quad 0 \leq x, \dot{x}_m \leq L, \quad 1 \leq m \leq N$$

$$(3)$$

$$\frac{\partial \rho}{\partial x} \big|_{x=\dot{x}_m} = (k + \frac{V}{D})\rho(\dot{x}_m, t), \quad 0 \leq \dot{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0$$

$$\rho_t(x, \dot{x}_m, t) = D\rho_{xx}(x, \dot{x}_m, t), \quad 0 < x, \dot{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0$$

$$\rho(x, \dot{x}_m, 0) = f(x, \dot{x}, 0), \quad 0 < x, \dot{x}_m \leq L, \quad 1 \leq m \leq N$$

$$(4)$$

$$\rho(\dot{x}_m, t) = 0, \quad 0 < \dot{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0$$

The set (4) is the ideal trap problem in which no external field is present as may be realized from the absence of $k$ and $V$. The set (3) is the imperfect trap problem which includes the external field and its initial condition contains only the first term of the corresponding condition of the general set (2). The solution of (2) may be written as in [9, 10] (see Eq (4) there),

$$\rho(x, \dot{x}_m, t) = A\rho_1(x, \dot{x}_m, t) + B\rho_2(x, \dot{x}_m, t), \quad 0 \leq x, \dot{x}_m \leq L,$$

$$1 \leq m \leq N, \quad t > 0$$

$$(5)$$
where $\rho_1(x, \dot{x}_m, t)$ is the solution of the initial and boundary value problem of the set \([9, 10]\) and $\rho_2(x, \dot{x}_m, t)$ is that of \([9, 10]\). The ideal trap problem of \([9, 10]\) is the same as that discussed in \([9, 10]\) so, following the discussion there, we write for $\rho_2(x, \dot{x}_m, t)$

$$
\rho_2(x, \dot{x}_m, t) = \sin\left(\frac{\pi x}{\dot{x}_m}\right) \exp\left(-\frac{Dt\pi^2}{2\dot{x}^2_m}\right), \quad 0 \leq x, \dot{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0
$$

(6)

Regarding $\rho_1(x, \dot{x}_m, t)$ we may follow Condat et al \([8]\), which discuss the problem \([8]\) for the single trap at the origin, and write the solution for the multitrap case as

$$
\rho_1(x, \dot{x}_m, t) = \exp\left(\frac{V(x - \dot{x}_m)}{2D}\right) - \frac{V^2 t}{4D} \left(\frac{e^{-\frac{(x - \dot{x}_m)^2}{4Dt}}}{\sqrt{\pi Dt}} - (k + \frac{V}{2D}) \cdot \exp(Dt(k + \frac{V}{2D})^2 + (k + \frac{V}{2D})(x - \dot{x}_m)) \text{erfc}\left(\frac{(x - \dot{x}_m)}{2\sqrt{Dt}} + (k + \frac{V}{2D})\sqrt{Dt}\right)\right),
$$

(7)

$$
0 < x, \dot{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0,
$$

where $\text{erfc}(x)$ is the complementary error function defined as \([25]\) $\text{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-u^2} du$.

In order to adapt the general solution \([5]\) to the bounded $N$ multitrap system we may use, as in \([9, 10]\), either the $N$ (2X2) transfer matrices method \([20, 21]\) or the equivalent single (4N×4N) transfer matrix formalism. We use in this section the $N$ (2X2) transfer matrices method for $V \neq 0$ and write the general matrix equation \([9, 10]\)

$$
\begin{pmatrix}
A_{2N+1} \\
B_{2N+1}
\end{pmatrix} = T(a + b)T(\frac{(N - 1)(a + b)}{N})T(\frac{(N - 2)(a + b)}{N})\ldots
$$

(8)

$$
\ldots T(\frac{n(a + b)}{N})T(\frac{(n - 1)(a + b)}{N})\ldots T(\frac{2(a + b)}{N})T(\frac{a + b}{N})
\begin{pmatrix}
A_1 \\
B_1
\end{pmatrix},
$$

where the $A$’s and $B$’s are respectively the coefficients of the imperfect and ideal trap components from Eq \([5]\). The $N$ $T$’s in Eq \([8]\) are all two-dimensional transfer matrices that differ from each other by the value of $x$ only \([9]\). Thus, a representative one which relates the two faces of the same trap that are located, for example, at $x = x_1$ and $x = x_2$, where $x_2 > x_1$, may be written as \([9, 10]\)

$$
T(x_1, x_2) = \begin{pmatrix}
T_{11}(x_1, x_2) & T_{12}(x_1, x_2) \\
T_{21}(x_1, x_2) & T_{22}(x_1, x_2)
\end{pmatrix},
$$

(9)

where \([9, 10]\)

$$
T_{11}(x_1, x_2) = \frac{\alpha(D_o, x_1, t)\alpha(D_i, x_2, t)}{\alpha(D_i, x_1, t)\alpha(D_o, x_2, t)}
$$

(10)
\begin{equation}
T_{12}(x_1, x_2) = 0
\end{equation}

\begin{equation}
T_{21}(x_1, x_2) = \frac{\eta(D_i, x_2, t)}{\eta(D_i, x_1, t)} \left( \frac{\xi(D_o, x_1, t)}{\eta(D_i, x_1, t)} - \frac{\alpha(D_o, x_1, t)\xi(D_i, x_1, t)}{\alpha(D_i, x_1, t)\eta(D_i, x_1, t)} \right) + \frac{\alpha(D_o, x_1, t)}{\alpha(D_i, x_1, t)} \left( \frac{\xi(D_i, x_2, t)}{\eta(D_o, x_2, t)} - \frac{\alpha(D_o, x_2, t)\xi(D_i, x_2, t)}{\alpha(D_o, x_2, t)\eta(D_o, x_2, t)} \right)
\end{equation}

\begin{equation}
T_{22}(x_1, x_2) = \frac{\eta(D_o, x_1, t)\eta(D_i, x_2, t)}{\eta(D_i, x_1, t)\eta(D_o, x_2, t)}
\end{equation}

The parameters \( \alpha, \xi, \) and \( \eta \) are given by (compare with the \( V = 0 \) case in Eqs (10)-(13))

\begin{equation}
\alpha(D, x, t) = \rho_2(x, t) = \exp\left( \frac{V(x - \dot{x}_m)}{2D} - \frac{V^2}{4D} \right) \left( \frac{e^{-\frac{(x-x_m)^2}{4Dt}}}{\sqrt{\pi Dt}} - (k + \frac{V}{2D}) \cdot \exp(Dt(k + \frac{V}{2D}))^2 + (k + \frac{V}{2D})(x - \dot{x}_m) \right) \cdot \text{erfc}\left( \frac{(x - \dot{x}_m)}{2\sqrt{Dt}} + (k + \frac{V}{2D})\sqrt{Dt} \right)
\end{equation}

\begin{equation}
\xi(D, x, t) = \frac{\partial \alpha(x, t)}{\partial x} = \exp\left( \frac{V(x - \dot{x}_m)}{2D} - \frac{V^2}{4D} \right) \left( \frac{e^{-\frac{(x-x_m)^2}{4Dt}}}{\sqrt{\pi Dt}} - (k + \frac{V}{2D})^2 \cdot \exp(Dt(k + \frac{V}{2D}))^2 + (k + \frac{V}{2D})(x - \dot{x}_m) \right) \cdot \text{erfc}\left( \frac{(x - \dot{x}_m)}{2\sqrt{Dt}} + (k + \frac{V}{2D})\sqrt{Dt} \right)
\end{equation}

\begin{equation}
\eta(D, \dot{x}_m, t) = -\frac{\pi}{\dot{x}_m} e^{-\frac{(\dot{x}_m)^2}{4Dt}}
\end{equation}

In order to find the density \( \rho(x, \dot{x}_m, t) \) from Eq (5) at each point \( x \) in the multitrapping system we have to determine the coefficients \( A \) and \( B \) of the imperfect and ideal trap components at this point. If, for example, this point happens to fall at the \( m \)-th trap then one has to multiply \( m \) transfer matrices each of the kind given by Eqs (10)-(13). We denote the components of the two-dimensional matrix that results from such a product by \( T_{m11}, T_{m12}, T_{m21} \) and \( T_{m22} \) and those of any one of the multiplied \( m \) matrices by \( T_{11}(l), T_{12}(l), T_{21}(l) \) and \( T_{22}(l) \) where \( 1 \leq l \leq m \). Thus, as realized from Eqs (10)-(13) (and from (10) for \( V = 0 \)), the components \( T_{N11}, T_{N12}, T_{N21} \) and \( T_{N22} \) may be expressed recursively as

\begin{equation}
T_{N11} = T_{(N-1)11} T_{11}(N) = \ldots = T_{11}(N) T_{11}(N - 1) \ldots T_{11}(2) T_{11}(1)
\end{equation}

\begin{equation}
T_{N12} = T_{(N-1)12} = \ldots = T_{212} = T_{12}(1) = 0
\end{equation}

\begin{equation}
T_{N21} = T_{(N-1)21} T_{21}(N) + T_{(N-1)11} T_{21}(N)
\end{equation}

\begin{equation}
T_{N22} = T_{(N-1)22} T_{22}(N) = \ldots = T_{22}(N) T_{22}(N - 1) \ldots T_{22}(2) T_{22}(1)
\end{equation}
It is found that the component $T_{N_{11}}$ tends to unity for growing values of the variables $N$ or (and) $c$. That is, the larger is either the number of traps or the intervals among them (or both) the higher is the tendency of the component $T_{N_{11}}$ to unity. Note that the same result have been found also in [9] for $V = 0$ with respect to the same variables $N$ and $c$ (see the discussion there after Eq (30)). We also find regarding the variable $V$ that the lower its value is the smaller becomes $T_{N_{11}}$. The same result is obtained also for negative $V$. We also find that $T_{N_{11}} \to 0$ for growing values of the total length $L$ and tends to unity for small values of it. Also, $T_{N_{11}}$ increases for larger values of either the time $t$ or $\dot{x}_m$.

Regarding the component $T_{N_{22}}$ we find that it does not assume values outside the range $(0, 1)$. Also, its factors $T_{22}$ satisfy $\lim_{N \to \infty} T_{22} = 0$ for $x \approx 0$ and $\lim_{N \to \infty} T_{22} = 1$ for $x \approx L$ (see in [9] Eq (26) and the unnumbered equation after Eq (27)). Thus, at large $N$, the product $T_{N_{22}}$ also tends to either unity or 0. We also find for small $c$ that the larger is either the number of traps $N$ or the time $t$ the more apparently $T_{N_{22}}$ tends to zero and this holds also for small values of $L$. When, however, $c$ increases $T_{N_{22}}$ clearly tends to unity. Note that $T_{N_{22}}$ does not depend upon the variable $V$ as seen from Eqs (13) and (16).

The component $T_{N_{21}}$ may generally have any value from $(-\infty, +\infty)$ but there are specific ranges of $N, L, c, V, k$ and $t$ for which $T_{N_{21}}$ tends to zero. Thus, it is found for growing $c$ that $T_{N_{21}}$ decreases fastly to zero if the increasing values of $c$ are small and slowly if these values are large. For example, increasing $c$ in the range $20 \leq c \leq \infty$ causes $T_{N_{21}}$ to decrease so slowly that it may be regarded as almost constant over this range. We find that $T_{N_{21}}$ assumes very high values for either large $N$ or small $L$ but when $L$ grows to a value which is comparable to that of $N$ the component $T_{N_{21}}$ may even decrease to zero. It is also found that the larger is $V$ the smaller become the corresponding values of $T_{N_{21}}$. For example, for $V \geq 24$ $T_{N_{21}}$ assumes very small values of the order of $10^{-11}$ but when $V$ decreases below 20 the value of $T_{N_{21}}$ becomes very large. Negative values of $V$ have similar effect on $T_{N_{21}}$ as the corresponding positive ones. Also, $T_{N_{21}}$ increases for larger values of the time $t$ and decreases for small $\dot{x}_m$.

We, thus, find that there are ranges of $N, L, c, V, k$ and $t$ for which the components of the total matrix $T_N$, that result from the $N$ products at the right hand side of Eq (8), assume the values of $T_{N_{11}} = 1, T_{N_{21}} = 0$ and $T_{N_{22}} = 1$. In this case all the diffusing particles pass through all the traps in which case the transmission is maximal. That is, the ideal and
imperfect trap components of the initial density do not change by the presence of either the traps or the fields (or both) in which case the product of the $N$ transfer matrices at the right hand side of Eq (8) results in the two-dimensional unity matrix. This is seen in Figure 1 which is composed of the three Panels $A - C$ which respectively show three-dimensional surfaces of the components $T_{N_{11}}, T_{N_{21}}$ and $T_{N_{22}}$ as functions of $c$ and $N$. All the three Panels are drawn for $V = 15, k = 1, D_o = 0.8, D_i = 0.4, t = 1$ and $L = 5$ and for the same ranges of $15 \geq N \geq 1$ and $300 \geq c \geq 20$. Panel $A$ shows the component $T_{N_{11}}$ and one may see that for large values of $c$ and $N$ $T_{N_{11}} \to 1$. The same result is obtained also in Panel $C$ for the component $T_{N_{22}}$ whereas in Panel $B$ we see that for large values of $c$ and $N$ the component $T_{N_{21}}$ tends to zero. Thus, substituting these values in Eq (8) and using the fact that one always have \[ T_{N_{12}} = 0 \] we obtain

\[
\begin{pmatrix}
A_{31} \\
B_{31}
\end{pmatrix} =
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
\begin{pmatrix}
A_1 \\
B_1
\end{pmatrix},
\]

That is, all the particles that approach the multitrap system pass through it without any decrease in either the ideal or the imperfect trap components of the density. Note that for $V = 0$ we have shown in \[9\] this unity value of the transmission for the imperfect trap component of the density (see Eq (28) there) and the same result is obtained in \[10\] for the ideal trap component.

III. THE ENERGY ASSOCIATED WITH THE BOUNDED MULTITRAP SYSTEM

We, now, discuss the energy associated with the diffusing particles in the presence of an external field. We do this by following the conventional discussion one may find in the literature regarding diffusive systems in the absence of external fields (see, for example, [24]). The presence of the field introduces an additional source of energy (besides that related to the diffusion through the traps) which must be taken care of by adding an extra term (to the kinetic energy) that depends upon the velocity $V$. We, thus, assume that the total energy is composed of two parts: kinetic and potential where the former results from the diffusive motion and the external field and the later from the presence of the traps. In the absence of any external field the particles diffuse with an average diffusion velocity $\bar{v}_D$ given, for the one-dimensional case, by \[24\] $\bar{v}_D = \sqrt{\frac{2D}{t}}$ where $D$ is the diffusion constant. Note that since
the two densities inside and outside the traps satisfy \( D_i \neq D_o \) then also the diffusion velocity \( \bar{v}_D \) and the general density \( \rho \) from Eq (3) satisfy \( \bar{v}_D \neq \bar{v}_D_o \) and \( \rho D_i \neq \rho D_o \). As remarked, the natural diffusive motion for \( V = 0 \) is towards the positive \( x \) axis so when a field is present and points in that direction it accelerates the motion of the particles or decelerates it if it is oppositely directed. Thus, we may write the kinetic energy of the diffusing particles as

\[
E_{K,V \neq 0}(x, \dot{x}_m, t) = \frac{1}{2} \rho(x, \dot{x}_m, t)(v_D^2 \pm V^2) = (A \rho_1(x, \dot{x}_m, t) + B \rho_2(x, \dot{x}_m, t)) \cdot \left( \frac{D}{t} \pm \frac{V^2}{2} \right), \quad 0 \leq x, \dot{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0, \tag{19}
\]

where \( \rho_2(x, \dot{x}_m, t) \) and \( \rho_1(x, \dot{x}_m, t) \) are given by Eqs (3)-(7). \( V \) is, as remarked, the velocity that results from the external field and the plus and minus signs in front of \( \frac{V^2}{2} \) denote respectively that the kinetic energy due to the field is either added for \( V > 0 \) or subtracted when \( V < 0 \) from that due to \( \bar{v}_D \). Note that for large \( t \) the kinetic energy from the last equation becomes zero since in this case both \( \rho_1 \) and \( \rho_2 \) vanishes as realized from Eqs (3)-(7).

By following the conventional discussion of the energy in classical diffusive systems [24] we may conclude that the force that acts on the particles is related to the potential energy which originates from the presence of the traps. This force is assumed to be proportional to the trapping rate \( k \) so for very large \( k \) (ideal traps) it assumes maximal values and for \( k = 0 \) (absence of traps) it vanishes. Also, since we have always assigned throughout this work a rather small value of unity for \( k \) which means that the imperfect traps have weak influence upon the particles we correspondingly assume an inverse proportionality of the force to the squared distance of the particles from the traps. This means, as remarked, that the particles feel the effect of the traps only at small distances from the traps. Thus, one may write the force on any particle that results from the trap as \( F(x, \dot{x}_m) = -\frac{gk}{(x - \dot{x}_m)^2} \), where \( g \) is the proportionality constant and the minus sign indicates an attractive force. Thus, assuming that each trap serves as a central force source one may find the potential energy from

\[
E_P(x, \dot{x}_m) = -\int_{(x - \dot{x}_m)}^{(x - \dot{x}_m)} F(x, \dot{x}_m) dx = -\int_{(x - \dot{x}_m)}^{(x - \dot{x}_m)} \left( -\frac{gk}{(x - \dot{x}_m)^2} \right) dx =
\]

\[
= -gk \left( \frac{1}{x - \dot{x}_m} - \frac{1}{x_r - \dot{x}_m} \right) = -gk \left( \frac{1}{(x - \dot{x}_m)} \right), \tag{20}
\]

where we assume that the reference point \( x_r \) is at infinity. Thus, we may write the total
energy of the diffusing particles in the presence of field as

\[ E_{\text{total}(V \neq 0)}(x, \dot{x}_m, t) = E_{K(V \neq 0)}(x, \dot{x}_m, t) + E_P(x, \dot{x}_m) \]

\[ 0 \leq x, \dot{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0, \]

where \( E_{K(V \neq 0)}(x, \dot{x}_m, t) \) and \( E_P(x, \dot{x}_m) \) are given respectively by Eqs (19) and (20). In the absence of an external field the total energy is

\[ E_{\text{total}(V = 0)}(x, \dot{x}_m, t) = E_{K(V = 0)}(x, \dot{x}_m, t) + E_P(x, \dot{x}_m) = \frac{1}{2} \rho_{V=0}(x, \dot{x}_m, t) \ddot{v}_x^2 + \]

\[ + E_P(x, \dot{x}_m) = \frac{1}{2}(A\rho_{V=0}(x, t) + Bp_2(x, \dot{x}_m, t)) \cdot \frac{D}{t}, \]

\[ 0 \leq x, \dot{x}_m \leq L, \quad 1 \leq m \leq N, \quad t > 0, \]

where \( \rho_{1V=0} \) is the imperfect trap component of the density for \( V = 0 \) and is given as \( \rho_{1V=0} = \text{erf}(\frac{x}{2\sqrt{Dt}}) + \exp(k^2Dt + kx) \cdot \text{erfc}(k\sqrt{Dt} + \frac{x}{2\sqrt{Dt}}) \) (see Eq (6) in [9]). \( p_2(x, \dot{x}_m, t) \) and \( E_P(x, \dot{x}_m) \) are given respectively by Eqs (6) and (20). The coefficients \( A \) and \( B \) in the last two equations are numerically determined in this section from the single \((4NX4N)\) matrix method (see the discussion after Eq (29) in [9]).

We now show that increasing \(|V|\) by even a small amount may change the energy in such an unexpected manner that it results, as seen in the following section, in a phase transition of the corresponding specific heat \( C_h \). This may realized form Panels A-D of Figure 2 which all show three dimensional surfaces of the energy \( E \) as function of \( x \) and \( c \). Panels A and B are both drawn for \( N = 2, \dot{x}_m = \frac{Lc}{N(1+c)}, k = t = g = 1, L = 30, D_o = 0.8, D_i = 0.4, 20 \geq c \geq 0.5, 40 \geq x \geq 0 \) and differ by the value of \( V \) which is 2 for Panel A and 5 for B. Thus, by comparing between them one may realize that increasing \( V \) by only 3 units causes to a disproportionally large increase of \( E \) from \(|E| \approx 12 \) in Panel A to \( E \approx 14000 \) in B. This large jump of the energy entails a corresponding discontinuous change in the values of the specific heat \( C_h \) which implies, as will be shown, that it goes through a phase transition. The same result is obtained also for negative \( V \) but compared to \( V > 0 \) the changes obtained are larger and found at smaller values of negative \( V \). This may be seen in Panels C and D of Figure 2 which are both drawn for \( N = 5, \dot{x}_m = \frac{2Lc}{N(1+c)} + \frac{L}{N(1+c)}, k = g = t = 1, L = 30, D_o = 0.8, D_i = 0.4, 20 \geq c \geq 0.5, 40 \geq x \geq 0 \) and differ by \( V \) which is \(-0.5 \) for Panel C and \(-0.8 \) for D. Thus, by comparing these two Panels one may realize that decreasing \( V \) by only three tenths from \(-0.5 \) to \(-0.8 \) results in a giant
change of the energy from $|E| \approx 10$ in Panel $C$ to $E \approx 10^8$ in $D$. This entails, as will be shown in the following section, a corresponding phase transition of the specific heat $C_h$. One may explain these large changes of the energy by reasoning that increasing the intensity of the field $|V|$ beyond some limit causes the particles to overcome any resistance related to the diffusion in the presence of traps. Thus, their energy increases disproportionally to the change of $|V|$ that causes it. A similar behaviour is encountered in Laser tubes [27] when the pumping energy (field) attains a limit value which causes the intensity of the produced light to increase in a phase transitionsal manner.

It is expected, regarding the dependence of the energy upon the trapping rate $k$, that the larger $k$ becomes the more controlled will be the diffusing particles by the traps in which case the kinetic (and the total) energy of these particles decrease. This is shown from recalling that for $N = 2, \ V = 5, \ k = 1, \ t = g = 1, \ L = 30, \ D_o = 0.8, \ D_1 = 0.4, \ \dot{x} = \frac{L_c}{N(1+c)}$, $20 \geq c \geq 0.5$ and $40 \geq x \geq 0$ we have obtained that the larger values of the energy are $E \approx 14000$. Now, it have been, numerically, found (not shown) that if $k$ is raised from $k = 1$ to $k = 5$, keeping the values of all the other parameters as before, the larger values of the energy are decreased to $E \approx 8000$. When $k = 10$ we find that $E \approx 5000$ and for $k = 15$ the larger $E$ further decrease to $E \approx 3000$. A similar behaviour of decreasing energies for larger $k$ is found also for negative $V$.

IV. SINGLE AND DOUBLE-PEAK PHASE TRANSITION IN THE SPECIFIC HEAT OF THE BOUNDED MULTITRAP SYSTEM

The average energy from which one may derive most of the statistical mechanics variables such as the specific heat $C_h$, the free energy $F$, the entropy $S$ etc may be written as

$$<E_{total}> = \frac{\sum E_{total} e^{-\beta E_{total}}}{\sum e^{-\beta E_{total}}},$$

where $\beta = \frac{1}{k_b T}$, $k_b$ is the Boltzman constant and $T$ is the temperature in Kelvin units. Substituting in the former equation the appropriate expression for $E_{total}$ from Eq (21) or (23) yields respectively the average energy for the presence or absence of an external field. From the expression of the average energy $<E_{total}>$ we obtain the specific heat $C_h$

$$C_h = \frac{\partial <E_{total}>}{\partial T} = \frac{\partial}{\partial T} \left( \frac{\sum E_{total} e^{-\beta E_{total}}}{\sum e^{-\beta E_{total}}} \right) = \frac{1}{T^2} \left( <E_{total}^2> - <E_{total}>^2 \right) \quad (23)$$
Figure 3 shows a three dimensional surface of $C_h$ from Eq (23) as function of the ratio $c$ and the temperature $T$ where no external field is present in which case the appropriate energy to be substituted in the last equation is that from Eq (22). Figure 3 is drawn for $N = 2$, $k = 1$, $L = 30$, $t = 1$, $g = 1$, $x_m = \frac{Lc}{N(1+c)}$, $20 \geq c \geq 0.5$ and $10 \geq T \geq 0.1$. As seen, the height of the surface for $C_h$ increases with growing values of the ratio $c$ until some maximum (not shown in the figure). One may also realize that at small values of $c$ and $T$ the surface of $C_h$ jumps upward to its local maximal values from which it descends in a similar manner to zero. These local maxima are seen to be arrayed along horizontal lines which form, in relation to their neighbouring lines, a sharp edge which becomes widened and flattened as $c$ grows.

The specific heat $C_h$ is certainly undifferentiable at the sharp edge so it goes through phase transition at these points [13, 26]. We calculate at the following the critical exponents $\chi$ [26] associated with this and other discontinuities of $C_h$. We find that increasing $N$ or $k$ or $g$, while keeping the values of the other parameters constant, does not cause to any change in the form of $C_h$ shown in Figure 3 except to its translation from its position along the $c$ axis to a one that tends to be aligned along the $T$ axis. That is, the same surface of $C_h$ is rotated in the $c-T$ plane for growing values of $N$ or $k$ or $g$. If, on the other hand, the value of the total length $L$ is simultaneously increased with that of $N$ then the remarked rotation of the surface of $C_h$, obtained for large values of $N$, is avoided and this surface remain in its form and place. Unlike the case of $V \neq 0$, to be discussed in the following, we find for $V = 0$ that except for the remarked points of discontinuity associated with smaller values of $c$ and $T$ there are no other points at which $C_h$ becomes discontinuous.

We discuss now the specific heat $C_h$ obtained when an external field is included with each trap. It is found, as for the $V = 0$ case, that the corresponding curves of the specific heat $C_h$ jumps abruptly from zero for small $c$ and $T$ to their maximal values from which they similarly descend to zero. Also, as for Figure 3, these maximal values are arranged along lines which form a sharp edge for small $c$ and $T$ which become widened and flattened as $c$ increases. The specific heat function is clearly undifferentiable along the sharp edge which implies, as for the $V = 0$ case, that it goes through phase transition [13, 26] at these points. But, in contrast to the former case, there exist other points, not at small values of $c$, for which the specific heat goes through phase transition. This is demonstrated in Figure 4 which is drawn for $V = 5$, $N = 2$, $k = g = t = 1$, $L = 30$, $x_m = \frac{Lc}{N(1+c)}$ and which is related not only
to the more obvious discontinuity of the two spiky columns at small $c$ and $T$ but also to that of the apparently continuous surface at large $c$’s. This is clearly shown in Figure 5 in which we isolate from the surface of Figure 4 four curves of the specific heat $C_h$ as function of the temperature $T$ for $c = 3, 3.1, 3.2, 3.3$. One can see that each curve of the four shown assumes the form of two inverted and indented tooth which are clearly undifferentiable and so they constitute a double-peak phase transition. We thus see, as remarked, that the unexpected large change in the values of the energy in Panel $B$ of Figure 2, which is drawn for the same values of $V, N, k, L, g, t,$ and $\dot{x}_m$ as those of Figures 4-5, is affected through the double peak phase transition of the corresponding specific heat of Figure 5. This depends, as noted, upon the value of $\dot{x}_m = \frac{Lc}{N(1+c)}$, so we expect that changing its value may result in finding double peaks phase transitions at other values of $c$ and $N$. This is indeed the case as we find (not shown here), for example, for $N = 4, 10.6 \geq c \geq 10$ and $\dot{x}_m = \frac{2Lc}{N(1+c)} + \frac{L}{N(1+c)}$, which is the location of the left hand face of the second trap.

From the former discussion we see that for positive values of $V$ there is associated a single peak for the smaller values of $c$ and a double peak for some higher values of it. When we consider, however, negative values of $V$ we find that the double peaks generally emerge for the smaller values of $c$. This is demonstrated in the right hand Panel of Figure 6 which shows 2 curves of the specific heat $C_h$ as function of the temperature $T$ for $V = -1.92, g = k = t = 1, L = 30, D_o = 0.8, D_i = 0.4, \dot{x}_m = \frac{Lc}{N(1+c)}$ and for the two values of $c = 0.39, 0.4$. In this case the first peaks of the two curves are small compared to the seconds. The left hand Panel shows 8 double peaks curves of the specific heat as function of $T$ for $\dot{x}_m = \frac{2Lc}{N(1+c)} + \frac{L}{N(1+c)}, N = 5, V = -0.37, g = k = t = 1$ and $c = 1.5 + 0.065 \cdot n, \ n = 1, 2, \ldots, 7$. These phase transitions of $C_h$ correspond to the unexpected large change of the energy which is shown in Panels $C-D$ of Figure 2 for exactly these values of $c, N, t, g, k, \dot{x}_m$ and in the neighbourhood of $V = -0.5$. These Panels demonstrate, as remarked, that slightly changing the value of $V$ in the neighbourhood of $V = -0.5$ by only three tenths changes the larger values of the energy from $|E| \approx 10^1$ to $E \approx 10^8$. This change in the energy is demonstrated in the double peak phase transition shown in the left hand Panel of Figure 6. Note that all the eight first peaks, as well as all the second peaks, touch each other and seem as one curve. The appropriate energy to be associated with negative $V$ is that of the expression $\frac{V^2}{2}$ in which one should take, as remarked, the minus sign in front of $\frac{V^2}{2}$.

We may suggest an explanation for the occurrence of the mentioned large changes in
the energy which entail the corresponding discontinuous peaks in the specific heat $C_h$. We confine our attention to the discussed examples of $N = 2$ and $N = 5$ when one respectively changes from $V = 2$ to $V = 5$ and from $V = -0.5$ to $V = -0.8$. As remarked, the change of $V$ for $N = 2$ entails a change in the larger values of the energy from $E \approx 12$ to $E \approx 14000$. Looking at the expression (19) for $E$ one may realize that the large increase in $E$ results from a corresponding increase of the imperfect density $\rho_1$ from Eq (7) (the ideal density $\rho_2$ does not depend upon $V$ and so it does not change with $V$ (see Eq (6))). As seen from Eq (7) the dependence of $\rho_1$ upon $V$ is mainly exponential. Thus, when $V$ changes from 2 to 5 we find for the ratio $\rho_{1v=5}/\rho_{1v=2}$ the value of $\rho_{1v=5}/\rho_{1v=2} = 2.3096 \cdot 10^{12}$ where we use the same values used for all the other parameters that lead to Panels A and B of Figure 2. That is, the density for $V = 5$ has enormously grows in relation to that for $V = 2$. This is to be compared, for example, to water when one lower its temperature from the gaseous state to the liquid one in which case the density of the water molecules grows in a phase transitional manner. This behaviour is repeated when one continues to decrease the temperature to $0^0C$ from the liquid state to the solid one in which case the density of the water molecules increases again in a phase transition manner. We have mentioned in the previous section the example of laser tubes for which the intensity of light increases greatly when the pumping energy (corresponding to $V$ here) attains a specific value. This occurs because a macroscopic aggregate of atoms have been transferred by the pumping energy into the appropriate laser state \[11\]. A similar grow of the density occurs, as remarked, also here when one increases for $N = 2$ the velocity $V$ from 2 to 5.

The double peaks shown in Figure 6 which are associated with small negative $V$ may be explained by noting that the external diffusion constant employed here is $D_o$ is 0.8 (the internal diffusion constant is even lower $D_i = 0.4$). That is, when one turns on an external field which is directed opposite to the diffusive motion then when the value of this field becomes $V = -0.8$ it actually neutralizes and cancels the influence of the traps on the particles so that their energy becomes very large.

The appearance of the double peaks for these values of $V$ demonstrates further (more than the single peak) the large change that the density and the energy have passed through when $V$ changes as described. We must, however, note that these peaks depend not only upon $V$ but also upon the other parameters, such as $N$, $x_m$, $t$ etc, that control the behaviour of $E$. 
one may calculate the related critical exponents $\chi$ associated with these phase transitions by using the following equation in the neighbourhood of the critical temperature $T_c$

$$C_h(\epsilon) = A + B\epsilon^\chi,$$

where $\epsilon = \frac{T-T_c}{T_c}$ and $A, B$ are constant. The first order derivative of $C_h(\epsilon)$ diverges at $T = T_c$ so the critical exponent $\chi$ may be obtained from

$$\chi = 1 + \lim_{\epsilon \to 0} \frac{ln|\hat{C}_h(\epsilon)|}{ln(\epsilon)} = 1 + \lim_{\epsilon \to 0} \frac{ln\left|\frac{\partial C_h}{\partial \epsilon}\right|}{ln(\epsilon)},$$

where the unity term denotes the first order derivative $\hat{C}_h(\epsilon)$ of the specific heat with respect to $\epsilon$. The value of $\chi$ may be obtained by plotting the curve of $C_h(\epsilon)$ in the close neighbourhood of $T = T_c$ and one can see from Figures 3-6 that $\chi$ assumes different values. Thus, assigning to the constants $A, B$ the respective values of 0 and 1 and plotting, as remarked, the graphs of $C_h(\epsilon)$ in the immediate neighbourhood of the single peaks in Figure 3, which are located at small $c$ and $T$, one may calculate $\chi$, using Eqs (24)-(25), as $\chi \approx \frac{1}{2}$. This value changes with respect to the single peaks of Figure 4 which are also located at small $c$ and $T$. That is, repeating the same procedure one may obtain the value of $\chi \approx \frac{4}{3}$. For the eight first and second peaks in the left hand Panel of Figure 6 we find the respective values of $\chi \approx \frac{1}{3}$ and $\chi \approx \frac{1}{2}$. The $\chi$ of the double peaks of Figure 5 and also of the first peaks in the right hand Panel of Figure 6 is $\chi \approx \frac{1}{9}$.

Comparing the phase transition behaviour of the bounded one-dimensional multitrapping system to that of the corresponding quantum array of the bounded one-dimensional multibarrier potential [14] one may notice the following similarities and differences; The specific heats of both systems exhibit the same discontinuous jump at small values of $T$ and $c$ but whereas in the multitrapping system $C_h$ decreases, for growing values of $T$, to zero the corresponding quantum $C_h$ does not vanish but tends, for large $T$, to a finite value (see Figures 1-7 in [14]). Also, the phenomenon of the double peaks at which the specific heat $C_h$ is undifferentiable are discernable in both systems.

The variation of the critical exponent $\chi$ may be explained by noticing from Figures 3-6 that the different peaks shown in these figures correspond to different values of $N$ and $c$. Remembering that $N$ and $c$ respectively denote the number of traps and the ratio of their total interval to their total width one may realize that they, actually, control the shape and form of the multitrapping system. That is, Figures 3-6 with the different values of $N$
and $c$ actually correspond to different systems through which the particles pass and not
to different parameters of the same system. Thus, one may expect different values of the
critical exponent to be associated with these different systems. We note, however, that the
difference between these values is not large.

Using the expressions (21)-(22) for the energy one may obtain the other variables of
statistical mechanics. For example, the free energy $F$ is calculated, for either the presence
or absence of the external field, from \[ F = -k_b T \ln(\sum e^{-\beta E_{total}}). \] Using the last equation
one may write the entropy $S$ for the multitrap system
\[
S = -\frac{\partial F}{\partial T} = \frac{\partial}{\partial T}(k_b T \ln(\sum e^{-\beta E_{total}})) = k_b \ln(\sum e^{-\beta E_{total}}) + k_b \beta \frac{E_{total} e^{-\beta E_{total}}}{\sum e^{-\beta E_{total}}}
\] (26)
As for the specific heat $C_h$ one may draw $S$ for different values of the parameters $N$, $k$, $g$, $x_m$, $t$, $L$ and $c$. If, for example, we draw the surface of $S$ for exactly the same values of the
mentioned parameters as those of Figure 4 one may see (not shown here) two separate lobes
for small $c$ and $T$ which correspond to the two spiky columns of Figure 4.

V. CONCLUDING REMARKS

We have discussed the diffusion limited problem related to the bounded one-dimensional
imperfect multitrap system in the presence of external field $V$. The analytical methods
previously used \[9, 10\] to discuss the transmission of the particles through this system in
the absence of an external field were also used here in the presence of it. Thus, the $N (2X2)$
transfer matrices were used, as in \[6\], for discussing the transmission through the multitrap
system for $V \neq 0$ and the single $(4NX4N)$ transfer matrix for studying the energy and
the corresponding specific heat $C_h$. It has been found, as for the $V = 0$ case in \[9\], that
for certain values of the parameters associated with the system the transmission coefficient
\[9, 10\] of the diffusing particles tends to unity when $N$ and $c$ become large in which case
all the particles diffuse through all the traps. This has been shown not only for positive $V$
which pushes the particles towards the traps but also for negative values of it that repell
the particles towards the negative direction of the $x$ axis.

The unique characteristics of the multitrap system become more unexpected regarding
the energy of the diffusing particles in the presence of an external field. Thus, it has been
found that increasing $V$, for either positive or negative values of it, by even a small amount
results in a disproportionally large increase in the energy of the diffusing particles so that trying to calculate the related specific heat $C_h$ we find that it goes through phase transition. Moreover, for certain values of the parameters associated with the multitrap system, such as its total length $L$, the number of traps $N$, the ratio $c$, the time $t$, the location $x_m$ at which the particles are initially concentrated and the field $V$, one may find that the mentioned phase transition is demonstrated in the form of a double peak. The value of the related critical exponents associated with these phase transitions were found to vary between $\frac{1}{2}$ and $\frac{3}{5}$.

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FIG. 1: The three Panels A – C show three-dimensional surfaces of the components $T_{N_{11}}$, $T_{N_{21}}$ and $T_{N_{22}}$ from Eqs (17) as function of the ratio $c$ and the number of traps $N$ in the ranges of $300 \geq c \geq 20$ and $15 \geq N \geq 1$. The other variables are assigned the following values; $D_0 = 0.8$, $D_1 = 0.4$, $t = k = 1$, $L = 5$. The parameters $c$ and $N$ are obviously dimensionless and one may realize from Eqs (6)-(17) that the three components $T_{N_{11}}$, $T_{N_{21}}$ and $T_{N_{22}}$ are also dimensionless. As seen, the components $T_{N_{11}}$ and $T_{N_{22}}$ tend to unity for the larger values of $c$ and $N$ and the component $T_{N_{21}}$ tends to zero. This signifies that all the diffusing particles pass the multitrap system (see Eq (18)).
FIG. 2: Each of the four Panels shows a three-dimensional surface of the energy from Eq (21) as function of \( x \) and the ratio \( c \). The length \( x \) is given in units of cm, \( c \) is dimensionless and the energy \( E \) is given in units of ergs. Panels A – B are both drawn for \( N = 2, D_o = 0.8, D_i = 0.4, t = k = g = 1, L = 30, \) and \( x_m = \frac{Lc}{N(1+c)} \) but \( V = 2 \) for Panel A and \( V = 5 \) for B. Note that by increasing the value of \( V \) from 2 to 5 results in an unexpected large change of the energy from \( |E| \approx 10 \) to \( E \approx 14000 \). Similar results are shown in Panels C – D which are both drawn for \( g = k = t = 1, L = 30, D_o = 0.8, D_i = 0.4, N = 5 \) and \( x_m = \frac{2Lc}{N(1+c)} + \frac{L}{N(1+c)} \) but \( V = -0.5 \) for Panel C and \( V = -0.8 \) for D. Note the giant change from \( |E| \approx 18 \) in Panel C to \( E \approx 5 \cdot 10^8 \) in Panel D that results from slightly changing from \( V = -0.5 \) to \( V = -0.8 \). The negative values of \( E \) result from the negative potential energy.
FIG. 3: A three-dimensional surface of the specific heat $C_h$ from Eq (23) as function of the ratio $c$ and the temperature $T$ and in the absence of an external field. The units of $C_h$ and $T$ in this figure and in Figures 4-6 are [erg degree] and Kelvin degree respectively and $c$ is dimensionless. The appropriate expression for the energy substituted in Eq (23) is that from Eq (22). The figure is drawn for $N = 2$, $D_o = 0.8$, $D_i = 0.4$, $L = 30$, $k = g = t = 1$ and $\dot{x}_m = \frac{L e}{N(1+c)}$. Note the sharp edge of the surface for small $c$ and $T$ which becomes widened and flattened as $c$ increases.
FIG. 4: The specific heat $C_h$ from Eq (23) as function of $c$ and $T$. This Figure is drawn for $V = 5$, $N = 2$, $D_o = 0.8$, $D_i = 0.4$, $L = 30$, $k = g = t = 1$ and $\bar{x}_m = \frac{Lc}{N(1+c)}$. Note that these are the values for which Panel B of Figure 2 is drawn. From that Panel we see that changing the value of $V$ from 2 to 5 results in a large change of the energy. This change is demonstrated in the discontinuity of $C_h$ for either small $c$ as in here or for larger values of it as in Figure 5. The units of $C_h$ and $T$ are, as remarked, $\text{[erg/degree]}$ and Kelvin degree respectively and $c$ is dimensionless.
FIG. 5: The figure shows four different curves of the specific heat $C_h$ in units of $\frac{\text{erg}}{\text{degree}}$ as function of the temperature $T$ in units of Kelvin for $N = 2$, $V = 5$, $D_o = 0.8$, $D_i = 0.4$, $g = k = t = 1$, $L = 30$, $\tilde{x}_m = \frac{Lc}{N(1+c)}$ and for the following 4 values of $c$: $c = 3, 3.1, 3.2, 3.3$. The double peaks are clearly seen in each curve. Note that the spiky forms of Figure 4 are obtained for exactly the same values as in this figure except that $c$ is smaller. Thus, one may conclude from Figures 4-5 that for positive $V$ there exist single peaks for small $c$ and double peaks for the larger values of it.
FIG. 6: The two Panels show double peaks of the specific heat $C_h$ as function of $T$ for negative $V$ and $D_o = 0.8$, $D_i = 0.4$, $g = k = t = 1$, and $L = 30$. The Panel at the left shows eight double-peak curves for $N = 5$, $V = -0.37$, $\dot{x}_m = \frac{2Lc}{N(1+c)} + \frac{L}{N(1+c)}$ and the 8 values of $c = 1.5 + 0.065 \cdot n$, $n = 1, 2, \ldots 7$. The Panel at the right shows two double-peak curves for $N = 4$, $V = -1.92$, $\dot{x}_m = \frac{Lc}{N(1+c)}$ and the two values of $c = 0.39, 0.4$. $C_h$ and $T$ are given in units of $\frac{\text{erg}}{\text{degree}}$ and kelvin degree respectively.