Temperature fluctuations in a heat bath

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The model of two boxes in thermal contact each filled with an ideal quasiclassical gas is used to treat, in a unified way, temperature fluctuations in both finite and infinite heat baths. One box is regarded as the heat bath and the other serves as the thermometer.

I. INTRODUCTION

Several years ago Phillies[1] posed the following question: Given the measured value of a mechanical variable (for example, the total energy) of a thermometer in thermal equilibrium with a system, what is the temperature of that system and how well does the thermometer determine that temperature?

Phillies presented a critique of the standard treatment of temperature fluctuations which can be paraphrased as follows: Equilibrium statistical mechanics deals with systems in a canonical state in which, by definition, the temperature is *constant*; therefore, one cannot use the canonical ensemble to calculate temperature fluctuations. This motivated the introduction by him of a new ensemble called the "polythermal" ensemble, conceived as a collection of canonical ensembles with differing temperatures. Phillies used this ensemble to answer the question he posed. In this paper, the same question is asked and answered from a somewhat different perspective using the model of two boxes in thermal contact, each filled with an ideal quasiclassical gas of identical structureless particles.

A description of the ideal gas model can be found in any textbook on statistical mechanics.[2] Usually, however, these descriptions pertain to a subsystem connected to an infinite heat bath. Here, the model is developed so that one can treat the case of a thermometer connected to a finite heat bath. This is done in Sec. II, where the energy distribution function for the thermometer is derived. In Sec. III, the temperature fluctuations in a finite heat bath are calculated. Then, in Sec. IV, I consider what happens to the parameters of the system as the heat bath becomes very large, while the thermometer remains relatively small. This is followed, in Sec. V, by a discussion of the sense in which the temperature in an infinite heat bath may be said to fluctuate and a calculation of the magnitude of these fluctuations. The last section contains some general remarks.

II. THE ENERGY DISTRIBUTION FUNCTION FOR AN IDEAL GAS THERMOMETER

Consider two systems A_h and A in thermal equilibrium; A_h is the heat bath whose temperature is to be measured by system A, that is, the thermometer. Let the heat bath have a total energy E_h distributed amongst N_h structureless particles in a *cubical* box with volume V_h; the thermometer contains N particles with total energy E in a cubical box with volume V.[3] The combined system $A_h \oplus A$ is assumed to be thermally isolated and therefore its total energy $E_0 = E_h + E$ is a constant. In order to compute the statistical properties of the thermometer one needs its energy distribution function.

According to quantum mechanics the single-particle en-

ergy levels $E(n_x, n_y, n_z)$ of the heat bath and the thermometer are quantized:

$$E(n_x, n_y, n_z) = \epsilon (n_x^2 + n_y^2 + n_z^2),$$

with

$$\epsilon = h^2 / 8 M V^{2/3}; \tag{1}$$

therefore, the microstates of each system can be counted. Here, h is Planck's constant, M is the mass of a gas particle and n_x, n_y, n_z are positive integers. A *macrostate* of the gas is specified by the set of numbers $(E, V, N, \Delta E)$ where

$$E = \epsilon \sum_{\text{particles}} (n_x^2 + n_y^2 + n_z^2)$$

is the total energy of the gas and ΔE is a microscopically small interval about the total energy. In general, a given macrostate can be realized in a huge number of ways, each corresponding to a different microscopic arrangement of the gas particles. Let that number be $\Omega(E)$ for the thermometer and let $\Omega_h(E_h)$ be the corresponding number for the heat bath. In principle, the calculation of the statistical weight Ω would entail an enumeration of all the possible ways of making a constant sum out of the square of $3N$ integers. However, one can sidestep this combinatorial problem by observing that for the gas model the spacing between the energy levels will be extremely small for systems of macroscopic size.[4] The energy may therefore be treated as a continuous variable and Ω may be calculated accordingly. This calculation is outlined in the appendix where it is shown that

$$\Omega(E) = \frac{\pi \Delta E}{4\epsilon} \left(\frac{\pi E}{4\epsilon} \right)^{(3N/2) - 1} \Big/ \left[N! \, \Gamma \left(\frac{3N}{2} \right) \right]. \tag{2}$$

In general, one would not expect the microstates of the combined system $A_h \oplus A$ to occur with equal probability; however, it is a basic working hypothesis of statistical mechanics that when systems are in thermal equilibrium all microstates constrained to have the same energy E and which satisfy an additional set of macroscopic constraints (for example, fixed values of V and N) occur with equal probability.[5] A system for which this hypothesis holds true is called *microcanonical*. If, in fact, this hypothesis is true then the probability, $P(E)dE$, to find the thermometer with total energy lying in the interval $(E, E + dE)$ will be proportional to the total number of microstates of the combined system consistent with the energy of the thermometer lying in that interval, that is,

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$$P(E)dE = \text{const} \times \Omega(E) \times \Omega_h(E_h)dE,$$

$$= \text{const } E^{(3N/2)-1}(E_0-E)^{(3N_h/2)-1}dE. \qquad (3)$$

When normalized the energy distribution for the thermometer can be written as

$$P(E)dE = \frac{1}{B(m,n)}\left(\frac{E}{E_0}\right)^{n-1}\left(1-\frac{E}{E_0}\right)^{m-1}\frac{dE}{E_0}, \qquad (4)$$

where $B(m,n)$ is the beta function[6] and where, for simplicity, I have introduced the notation $n \equiv 3N/2$ and $m \equiv 3N_h/2$.

It should be emphasized that this distribution is valid for all sizes of the heat bath and of the thermometer. From it, all statistical mechanical properties of the model can be deduced.

III. TEMPERATURE FLUCTUATIONS IN A FINITE HEAT BATH

A basic assumption of this paper is that the temperature T is given by the formula

$$\frac{1}{T} \equiv \frac{\partial \ln \Omega(E)}{\partial E}. \qquad (5)$$

Other definitions of temperature, of course, exist; however, a survey of the standard textbooks on statistical mechanics reveals that the definition adopted here is the one most commonly used. One of the purposes of this paper is to examine some of the consequences of this definition for finite systems. The temperature, defined in this way, is measured in energy units. To obtain expressions in which the temperature is measured in degrees Kelvin one should substitute $K_B T$ for T, where K_B is Boltzmann's constant.[7]

It should be noted that according to this definition of temperature the latter can only be defined if $\ln\Omega$ may be regarded as a continuous function of the energy, but the definition does not require a system to contain, necessarily, a large number of particles. Using the result for Ω given in Eq. (2) and the definition, Eq. (5), leads to the expression

$$T = E/(n-1), \qquad (6)$$

for the temperature of the thermometer. For the heat bath one obtains,

$$T = E_h/(m-1) = E_0/(m-1) - E/(m-1). \qquad (7)$$

Equation (7) suggests the introduction of the new parameter, T_∞, defined by

$$T_\infty \equiv E_0/(m-1), \qquad (8)$$

which I shall refer to as the *canonical* temperature. In the following our attention shall be focused on the temperature of the heat bath. Some comments about the temperature of the thermometer will be made in the last section. In general, the temperature of the heat bath will fluctuate. Its moments, with respect to the density Eq. (4), are easy to calculate and are given by

$$\langle (T)^\alpha \rangle = (T_\infty)^\alpha B(m+\alpha,n)/B(m,n). \qquad (9)$$

In particular, the average temperature and variance are, respectively,

$$\langle T \rangle = T_\infty m/(m+n) \qquad (10)$$

and

$$\sigma_T^2 = \langle T \rangle^2 n/[m(m+n+1)]. \qquad (11)$$

At this stage the canonical temperature, T_∞, appears merely as the parameter which sets the scale for the average temperature. In fact, that quantity does have a broader significance; but to see this one must take the model to the thermodynamic limit.

IV. THE THERMODYNAMIC LIMIT

It is instructive to see what happens as the size of the heat bath grows to infinity, while the average temperature remains bounded. In the thermodynamic limit, $m \to \infty$, the average temperature and the variance become

$$\langle T \rangle = T_\infty, \quad \sigma_T^2 = 0. \qquad (12)$$

One observes two important points: (1) T_∞ is seen to be the temperature of an infinite heat bath; and (2) that temperature, T_∞, is constant. One may regard this quantity as an intrinsic property of a heat bath in that it defines, and characterizes, an infinite sequence of (progressively larger, and hotter) heat baths. Presumably, it is the canonical temperature T_∞, rather than the average temperature $\langle T \rangle$, which is the important physical quantity. Actually, it turns out that it is the inverse canonical temperature, $\beta_\infty \equiv 1/T_\infty$, which appears most naturally in the various expressions which follow; accordingly, the subsequent discussion will be in terms of β_∞.

Now the question arises as to how β_∞ is related to a canonical ensemble? One way to answer this question is to take the thermodynamic limit of the energy distribution function of the thermometer, that is, Eq. (4). To do so, one begins by rewriting Eq. (4) as

$$P(E)dE = \left(\frac{\Gamma(m+n)}{\Gamma(m)\Gamma(n)(m-1)^n}\right)\beta_\infty(\beta_\infty E)^{n-1}$$

$$\times [1-\beta_\infty E/(m-1)]^{m-1}dE.$$

By using Stirling's formula[8] one can show that when $m \to \infty$ the expression in the first set of brackets goes to $1/\Gamma(n)$; the limit of the expression in the second set of brackets is an exponential. Hence, in the limit of an infinite heat bath one obtains

$$P(E|\beta_\infty)dE = \beta_\infty(\beta_\infty E)^{n-1}\exp(-\beta_\infty E)dE/\Gamma(n), \qquad (13)$$

as the energy distribution of the thermometer. This is identical to Eq. (3.9) of Phillies' paper if one identifies β_∞ with the parameter β in that equation; that is, the parameter β_∞ is identified as the parameter which appears in the canonical distribution, from which Eq. (3.9) is ultimately derived. Equation (13) illustrates a general result, namely, that in the thermodynamic limit all details pertaining to a system are subsumed into a few physical quantities; here the inverse canonical temperature β_∞. The further away one is from the thermodynamic limit the greater is the amount of detail required to describe the statistical behavior of a system. The moments given by Eq. (9) afford an example of this: They show that to fully specify the state of a finite heat bath one must give both the number of particles in the heat bath and in the thermometer as well as the value of the quantity β_∞, whereas, as indicated by Eq.

(12), in the thermodynamic limit the heat bath is fully specified by the single quantity β_∞.

V. FLUCTUATIONS IN THE INFERRED VALUE OF THE PARAMETER β_∞

The title of this section may appear somewhat contradictory. After all, it has just been argued that the parameter β_∞ is a constant. So in what sense can it be said to fluctuate? To answer this question one notes that the value of β_∞ (or T_∞) must be inferred from the measurement of some mechanical quantity. Since the latter will fluctuate, so too will the inferred values of β_∞. The pertinent question to ask then is: To what accuracy can one assert that the temperature of the heat bath has such and such a value? Such a question clearly belongs to the realm of statistical inference, and I shall assume that the task here is to infer a value for β_∞ given that one knows the total energy of the thermometer.

The most general way to make statistical inferences is to treat all uncertainty probabilistically and to do so using Bayes' theorem.[9] Bayes' theorem, applied to the problem at hand, can be stated as follows: If $P(E|\beta_\infty)$ is the likelihood for the thermometer to have a total energy E given β_∞; $P(\beta_\infty|E)d\beta_\infty$ is the probability that the temperature parameter could have the value β_∞ given E (this is the probability of interest here, called the posterior probability), and $\Pi(\beta_\infty)d\beta_\infty$ is the prior probability over the parameter space of β_∞, then

$$P(\beta|E)d\beta = P(E|\beta)\Pi(\beta)d\beta \Big/ \int_a^b P(E|\beta)\Pi(\beta)d\beta,$$ (14)

in which, for simplicity, the subscript on β has been dropped. It will be understood, for the rest of the paper, that β really means β_∞ and likewise for T. It is assumed that β is defined in some interval $[a,b]$ determined by the form of the conditional probability $P(E|\beta)dE$, that is, Eq. (4)

This elegant formula provides a direct method of making inferences about the value of the parameter β. To use it, however, one must specify the prior probability distribution for that parameter; and herein lies the rub: By what set of principles is the form of the prior probability distribution to be derived? One could simply make the intuitive choice

$$\Pi(\beta)d\beta = d\beta.$$ (15)

In fact, one can interpret Phillies' use of the polythermal ensemble as a Bayesian inference procedure with the uniform prior distribution

$$\Pi(T)dT = dT.$$

While this is the obvious choice I shall argue that its use in this case is questionable. This is not to say that the use of a uniform prior distribution is incorrect but merely that the prior distribution may not be uniform in the parameter T.

It is surely reasonable to demand that one's conclusions, about the heat bath and the thermometer, not depend upon how the probabilities are parametrized: It ought not to matter whether one uses T, β, or any other quantity as the parameter. Therefore, if one were to use a uniform prior distribution for the temperature then, to be consistent, one would be obliged to use the prior

$$\Pi(\beta)d\beta = \frac{d\beta}{\beta^2},$$ (16)

for the parameter β. One could not choose the prior for β to be uniform because the prior cannot be uniform in both T and β simultaneously. The difficulty is that given that one is ignorant of the value of T and β, one has no reason to choose the prior to be uniform in T rather than in β or, for that matter, vice versa. Something is amiss and one needs a guiding principle to resolve the issue.

Jaynes[10] has proposed a principle by which prior probabilities can be derived. Briefly stated it is this: In the absence of any prior knowledge about the value of a parameter, other than a knowledge of the set of transformations with respect to which the problem is invariant, the prior probability distribution should exhibit the invariances of the problem. It is clear that the problem is invariant with respect to a change in the energy scale $E \rightarrow qE$, $\beta \rightarrow \beta/q$. Therefore, according to Jaynes $\Pi(\beta)d\beta$ should be invariant under the aforementioned transformation. This will be the case if

$$\Pi(\beta)d\beta = \frac{d\beta}{\beta},$$ (17)

which, if one transforms to the parameter T, implies

$$\Pi(T)dT = \frac{dT}{T}.$$ (18)

It should be noted that this prior distribution for T is consistent because it is precisely what one would have obtained by an application of Jaynes' principle to the problem had it been parametrized in terms of the temperature rather than in terms of β. Incidentally, the parameter for which the prior distribution will be uniform is $\lambda \sim \ln T$.

In terms of the parameter β the posterior probability is

$$P(\beta|E)d\beta = E\left(\frac{\beta E}{(m-1)}\right)^{n-1}\left(1 - \frac{\beta E}{(m-1)}\right)^{m-1}$$
$$\times \frac{d\beta}{(m-1)B(m,n)},$$ (19)

from which all questions about the value of β, or T, can be answered. Note the interesting duality between $P(\beta|E)d\beta$ and $P(E|\beta)dE$: One can go from one to the other by the interchange $\beta \leftrightarrow E$. The moments of β are readily calculated to be

$$\langle(\beta)^\alpha\rangle = [(m-1)/E]^\alpha B(m,n+\alpha)/B(m,n).$$ (20)

From this, one obtains

$$\langle\beta\rangle = [(m-1)/E][n/(m+n)],$$ (21)

as an estimate of the value of the temperature parameter β, while

$$\sigma_\beta^2 = \langle\beta\rangle^2 m/[n(m+n+1)],$$ (22)

quantifies the degree of uncertainty in the estimate $\langle\beta\rangle$. One sees again that these quantities depend upon the details of both the heat bath and the thermometer. However, for an infinite heat bath these quantities are determined by the size of the thermometer only:

$$\langle \beta \rangle = n/E,$$

$$\sigma_\beta^2 = \langle \beta \rangle^2/n. \tag{23}$$

It is noteworthy that the behavior of the ratio $\sigma_\beta/\langle \beta \rangle$ accords with one's expection:

$$\sigma_\beta/\langle \beta \rangle = 1/\sqrt{n}. \tag{24}$$

The corresponding ratio for the temperature T (really, T_∞) does not, however, behave quite so tidily:

$$\sigma_T/\langle T \rangle = 1/\sqrt{n-2}. \tag{25}$$

Recalling that $n = 3N/2$, one sees that the ratio is undefined for a thermometer containing one particle! However, one should be wary about drawing strong conclusions from this because the small n behavior of the above equations is influenced by the form of the prior distribution for β_∞ and T_∞. Phillies used a uniform prior distribution for T_∞ and, consequently, obtained a different small n behavior.

VI. CONCLUDING REMARKS

When two systems are in thermal equilibrium their temperatures are equal. Well, not quite; this depends upon the size of the systems. Consider averaging over the expression for the temperature of the thermometer, given in Eq. (6). This leads to the expression,

$$\langle T \rangle = T_\infty n(m-1)/[(n-1)(m+n)], \tag{26}$$

for the average temperature of the thermometer. This differs from that for the heat bath, Eq. (10), by an amount

$$\Delta T = T_\infty (m-n)/[(m+n)(n-1)]. \tag{27}$$

So while it is true that for thermometers and heat baths containing a large number of particles the difference in temperature between the two is negligible it is not necessarily so for small systems. This is yet another indication that thermodynamic reasoning applies strictly to systems containing a large number of degrees of freedom. It may be possible to apply the methods of thermodynamics to small systems; however, one needs to be extremely cautious.

Of course, the above results are a direct consequence of the particular definition of temperature used in this paper. Gibbs[11] who, at the turn of the century, treated the same topic addressed in this section argued that the definition, Eq. (5), is "imperfect."[12] It is imperfect, in his view, precisely because that definition leads to the above results. Gibbs observes that a perfect statistical mechanical analogue of the temperature, as understood in thermodynamics, is the quantity he calls the *modulus* (T_∞ in our notation) which appears in the canonical distribution. However, not all systems under study are canonical; therefore, Gibbs' observation leaves open the question of whether a temperature can be defined for systems which are far from the thermodynamic limit and, if so, how. One can argue that it is useful to have a general definition of temperature valid for all systems in statistical equilibrium. Moreover, one can differ with Gibbs and argue further that the only obligation of any such definition is that it agrees with the usual notion of temperature in the domain in which that notion arose, namely, thermodynamics.

If indeed the temperatures, as defined by Eq. (5), of two finite systems in thermal equilibrium are not quite equal then one must look for some other quantity to characterize the notion of equilibrium. This quantity will be more fundamental than the temperature, so defined, in that it will be equal for the two systems irrespective of their size. One such quantity is

$$\tau = T_\infty (m-1)/(m+n), \tag{28}$$

which is equal to 2/3 times the average energy per particle. (The quantity τ could be interpreted as yet another kind of temperature.) One can use it to write some expressions in a more symmetric manner; in particular, the average temperature of the heat bath and of the thermometer can be written as

$$\langle T \rangle = \tau m/(m-1) \tag{29}$$

and

$$\langle T \rangle = \tau n/(n-1), \tag{30}$$

respectively. It should be stressed that the quantities $\langle T \rangle, T_\infty$ and τ are distinct physical quantities. However, in the thermodynamic limit they lose their separate identities and become numerically identical.

ACKNOWLEDGMENTS

APPENDIX

Consider a gas consisting of N structureless, identical, particles. If $G(E)$ is the number of microstates of the gas with total energy $\leqslant E$ then, by definition,

$$\Omega(E) = G(E+\Delta E) - G(E). \tag{31}$$

Let dG_i be the number of states available to a single particle i with momentum in the interval $(p_i, p_i + dp_i)$; dG_i is given by the phase space volume divided by h^3, that is,

$$dG_i = V 4\pi p_i^2 dp_i/h^3, \tag{32}$$

where V is the volume of the enclosure containing the particle. For a gas of N particles $G(E)$ is given by

$$G(E) = \frac{1}{N!} \int_0^E dE' \left[\prod_{i=1}^N \int_0^\infty dG_i \right] \delta\left(E' - \sum_{j=1}^N \epsilon_j \right), \tag{33}$$

where $\epsilon_i = p_i^2/2m$ are the single-particle energies. The delta function is most easily treated by using the identity

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^\infty d\omega e^{i\omega x},$$

whereupon the expression for $G(E)$ becomes

$$G(E) = \frac{1}{N!} \frac{V^N}{h^{3N}} (2\pi)^N (2M)^{3N/2} \int_0^E dE' \frac{1}{2\pi i}$$

$$\times \int_{-\infty}^\infty i d\omega e^{i\omega E'} \prod_{j=1}^N \int_0^\infty d\epsilon_j \epsilon_j^{1/2} e^{-i\omega\epsilon_j}. \tag{34}$$

Each integral within the product sign contributes an amount $\Gamma(3/2)/(i\omega)^{3/2}$ to the integral over ω. The integral over ω, which has a pole of order $3N/2$ on the real axis, can be performed by contour integration after displac-

ing the pole a small positive amount δ off the real axis. At the end one takes the limit $\delta \to 0$. A final integration over E leads to

$$G(E) = (\pi E/4\epsilon)^{3N/2}/[N!\ \Gamma(3N/2+1)], \qquad (35)$$

where ϵ is defined in Eq. (1). From the definition of Ω, given in Eq. (31), one obtains Eq. (2), in which terms $O[(\Delta E/E)^2]$ have been dropped.

[a] Operated by Universities Research Association Inc., under contract with the U.S. Department of Energy.

[1] G. D. J. Phillies, "The polythermal ensemble: A rigorous interpretation of temperature fluctuations in statistical mechanics," Am. J. Phys. 52, 629–632 (1984).

[2] See, for example: F. Mandl, *Statistical Physics* (Wiley, London, 1971), pp. 168–194.

[3] A cubical box has the virtue of keeping the maths simple.

[4] For example, if one takes $V=1$ cm^3 and M to be the mass of molecular hydrogen then according to Eq. (1) $\epsilon=2\times10^{-18}$ eV. For particles with energies of order $K_B T$, where K_B is Boltzmann's constant and T is the temperature, one would expect the spacing between levels, at those energies, to be of order $\sqrt{\epsilon K_B T}$, that is, about 10^{-10} eV at room temperature.

[5] I would hazard a guess that a majority of scientists believe the hypothesis of equal *a priori* probabilities, if true, is ultimately a consequence of the laws of mechanics (presumably quantum mechanics). One must admit, however, in the light of Gödel's incompleteness theorem, the logical possibility that this hypothesis is true and yet not derivable as a theorem of mechanics.

[6] Murray R. Spiegel, *Mathematical Handbook* (McGraw-Hill, New York, NY, 1968), p. 103.

[7] With the introduction of K_B and using Boltzmann's definition of entropy $S=K_B\ln\Omega$ one obtains, from Eq. (7), the usual thermodynamic definition of temperature, namely $1/T=\partial S/\partial E$.

[8] Murray R. Spiegel, *Mathematical Handbook* (McGraw-Hill, New York, NY, 1968), p. 102.

[9] The use of Bayes' theorem in this way is called *Bayesian statistics*. The following reference provides a thorough account: H. Jeffreys, *Theory of Probability* (Clarendon, Oxford, 1939).

[10] E. T. Jaynes, "Prior probabilities," IEEE Trans. Sys. Sci. Cyb. SSC-4, 227–241 (1968).

[11] J. Willard Gibbs, *Elementary Principles in Statistical Mechanics* (Dover, New York, NY, 1960). See, in particular, Chap. 14. This book was first published by the Yale University Press in 1902.

[12] As an historical aside it should be noted that Gibbs regarded neither the microcanonical approach to statistical mechanics nor the definition, Eq. (5), as incorrect in any fundamental way. Indeed, in Chap. 14 of his book he acknowledges that many regard the microcanonical approach as both simpler and more natural than the one based upon the canonical distribution.

Nonuniqueness in the solutions of Newton's equation of motion

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In the case of singular forces, for which some of the higher derivatives do not exist at a given point, it is not generally true that Newton's equations of motion will give unique solutions for given initial conditions. In this paper, the motion of a particle in a one-dimensional conservative force field is considered. The necessary and sufficient conditions that ensure unique solutions are determined.

I. INTRODUCTION

It is generally believed that Newtonian mechanics is deterministic. Given sufficient initial conditions, it is expected that the equations of motion will lead to unique trajectories. However, this is not always true. Let us discuss a simple example. A single particle (of unit mass) moves in a one-dimensional force field given by $F(x)=x^{1/3}$. Its equation of motion is $\ddot{x}=x^{1/3}$. For the initial conditions $x=0$, $\dot{x}=0$ at $t=0$ there exist three solutions; $x=0$ and $x=\pm(1/6)^{3/2}\ t^3$. One might think that this peculiarity essentially arises due to the singularity of the force (the first derivative blows up at $x=0$). But consider another case of a singular force $F(x)=x^{4/3}$, for which the second derivative blows up at $x=0$. With the initial conditions $x=0$, $\dot{x}=0$ at $t=0$, we are led to the unique solution $x=0$. Here, the solution is unique in spite of the force being singular.

These examples show that in the case of singular forces,

for which some of the higher derivatives do not exist at a given point, it is not generally true that Newton's equation of motion will give unique solutions for given initial conditions. Here, we study the simple case of a single particle moving in a one-dimensional force field and arrive at the most general condition that is both necessary and sufficient for the existence of unique solutions.

For the case considered, the equation of motion is

$$\ddot{x}=F(x)=-\frac{dV}{dx}. \qquad (1)$$

From the mathematical point of view, Eq. (1), in general, constitutes a second-order nonlinear differential equation and the usually stated condition for the existence of unique solutions is that $F(x)$ satisfy the Lipschitz condition in the domain of interest.[1,2] As these conditions and the proof are not well known, we give a brief discussion in the Appendix. However, the Lipschitz condition is a sufficient but not a