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THE CLASSICAL *ADIABATIC CONSTANCY* OF PV^{γ} FOR AN IDEAL GAS, CAN BE SHOWN TO BE A QUANTUM MECHANICAL OCCURRENCE, WHICH YIELDS THE PARTICULAR VALUE OF THE *CONSTANT*, IN QUESTION

Tolga YARMAN[*], **Alexander L. KHOLMETSKII**[**] **ve Önder KORFALI**[***]

[*] Department of Engineering, Okan University, Akfirat, Istanbul, Turkey
& Savronik, Eskisehir, Turkey, tolgayarman@gmail.com
[**] Department of Physics, Belarus State University, 4 Nezavisimosti Avenue,
220030 Minsk, Belarus, khol123@yahoo.com
& Department of Engineering, Okan University, Akfirat, Istanbul, Turkey
[***] Galatasaray University, Ortaköy, Istanbul, Turkey, dkorfali@yahoo.com

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Abstract: In this paper we find a *full connection* between the long lasting macroscopic classical laws of gases and the quantum mechanical description of *non-interacting particles* confined in a box, thus constituting an ideal gas. In such a gas, the motion of each individual molecule can be considered to be independent of all other molecules, and the macroscopic parameters of an ideal gas, mainly, pressure *P* and temperature *T*, can be defined as simple average quantities based on individual motions of all molecules in consideration. It is shown that for an ideal gas enclosed in a macroscopic cubic box of volume *V*, an *alphanumeric expression* for the *Constant* appearing in the classical law of adiabatic expansion law, i.e. $PV^{5/3} = Constant$, can be derived based on quantum mechanics. Note that this constant has otherwise remained for centuries, as just an *abstract quantity* in the form of $P_1V_1^{5/3}=P_2V_2^{5/3}= P_3V_3^{5/3}$ written for different thermodynamic states, delineated through an adiabatic transformation. No one even seems to have thought that it may eventually have a particular expression. Physical implications of the result we disclose are discussed.

Keywords: Adiabatic transformation, Quatnum Mechanics, Special Theory of Relativity, Universal Matter Architecture.

KLASİK PV^{γ} *ADİABATİK SABİTLİĞİ,* İDEAL GAZ İÇİN, KUVANTUM MEKANİKSEL BİR OLGU OLUP, BU YOLLA SÖZ KONUSU SABİT, SOMUT OLARAK BELİRLENBİLMEKTEDİR

Özet: Bu makalede, asırlardır bilinen *gaz yasaları* ile, bir kapta hapsolmuş olup, birbirleriyle etkileşmede bulunmayan parçacıkların oluşturduğu *ideal gazın kuvantum mekaniksel tasviri* arasında, *bütünsel bir bağ* kurulmaktadır. Böylesi bir gazda, her bir parçacık, birbirinden bağımsız olarak ele alınabilmektedir. Bu durumda, gazın *basınç P, sıcaklık T* gibi, *makroskopik özellikleri,* gazı oluşturan parçacıkların, ayrı ayrı hareketlerinin, *basit birer ortalaması* niteliğinde hesaplanabiliyor olmaktadır. Burada, bu çerçevede, *V* hacmindeki bir küpte hapsolmuş ideal bir gazın, *adiabatik dönüşüm sürecini*, resmeden $PV^{5/3} = Sabit$, bağıntısında yer alan, *Sabit'in*, kuvantum mekaniği zemininde, *somut* olarak ifade edilebileceği, ortaya konmaktadır. Söz konusu sabitin, öteki türlü, *asırlardır,* birinden ötekine, *adiabatik* olarak geçilen, çeşitli haller için, $P_1V_1^{5/3}=P_2V_2^{5/3}= P_3V_3^{5/3}$ eşitliklerinin işaret ettiği *soyut bir büyüklük* olarak algılanmaktan öteye geçemediği, kaydolunmalıdır. Hemen hiç bir yerde, bahse konu sabitin, *belli bir ifadesinin* olabileceğinin sorgulandığna dair bir işaret, ayrıca, görülebiliyor, değildir. Türetimin sonuçları tartışılmaktadır.

Anahtar Kelimeler: Adiabatik Dönüşüm, Kuvantum Mekaniği, Özel Görelilik Kuramı, Evrensel Madde Mimarisi.

INTRODUCTION

Time to time, most of us, no doubt, just like many scientists of the 20th century, were puzzled with the question of finding a link between the *Boltzmann Constant k* and the *Planck Constant h*. We will see below that, this is actually a *vain effort.* Nevertheless, de Broglie already in his doctorate thesis has brilliantly applied his relationship *(associating a wavelength with the momentum of a moving particle)* to the statistical equilibrium of gases [de Broglie, 1925], but did not advance his idea, to see whether one can along such a line, obtain anything related to the law of gases, established long ago, in 1650.

Let us assume that, the gas is made of just one kind of molecules. The *Boyle-Mariotte law of ideal gas* is given, as usual, by

$$PV = n_m RT = kNT\,; \tag{1}$$

here P is the pressure of the gas, V the volume of the gas, T the temperature of the gas, n_m the number of *moles* the gas is made of, N the number of molecules making the gas; R=8.31 Joules /ºK is the *gas constant;* further

$$k = R / N_A \tag{2}$$

is the *Boltzmann Constant,* and N_A the *Avogadro number.*

The *kinetic theory of gases* allows us to derive the same *casing* as that of Eq.(1) via considering the momentum change of each molecule separately, when bouncing back, from a wall of the given container [Halliday, Resnick, Walker, 1997]. Assuming for simplicity *(though without any loss of generality)* a *cubic geometry;* one, through a simple averaging, obtains

$$PV = \frac{N}{3} m\overline{v^2} = \frac{2}{3} N\overline{E}\ , \tag{3}$$

where $\overline{E} = m\overline{v^2}/2$ being the average *translational energy of molecules,* each of mass *m;* $\overline{v^2}$ is the *mean square velocity,* to be associated with the *average molecule.*

For the sake of completeness, let us recall the classical derivation of Eq.(3). The force f_x exerted by the molecule of mass m and velocity $\boldsymbol{v}\{v_x, v_y, v_z\}$ on the wall in the plane *yz*, is given by Newton's second law $f_x = -\Delta p_x / \Delta t$, where $\Delta p_x = -2mv_x$ is the algebraic increase in the momentum, whilst the molecule bounces back from the wall, and $\Delta t = 2L/v_x$, L being the size of the container along the x-direction. Thus one has, $f_x = m{v_x}^2/L$. We can suppose that we deal with an *average molecule,* and all molecules behave as this average molecule, in the ideal gas of concern. Hence, summing over N molecules the gas is made of, we get the total force F_x exerted on the wall lying on the yz plane, as $F_x = N\frac{m\overline{{v_x}^2}}{L} = \frac{N}{3}\frac{m\overline{v^2}}{L}$; here, $\overline{v_x^2}$ is the *mean square velocity* along x-direction; note that, at the *equilibrium,* this latter quantity, can be assumed to be the same as the mean square velocities $\overline{v_y^2}$, and $\overline{v_z^2}$ that come into play along the other two directions; note also that the overall *mean square velocity* $\overline{v^2}$ is given by $\overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2}$; thus at the *equilibrium* one can as usual, write $\overline{v^2} = 3\overline{v_x^2}$.

The pressure P exerted by N molecules on the wall of concern, is thence $P = \frac{N}{3}\frac{m\overline{v^2}}{L^3}$, which is Eq. (3), along with V=L^3.

Now comparing Eqs. (3) and (1), one, as usual, derives

$$\overline{E} = \frac{3}{2} kT \cdot \tag{4}$$

Furthermore, Eq.(3) can naturally be written for the pressure p that would be built in the volume V, containing *just one molecule* of translational energy *E:*

$$pV = kT = \frac{2}{3} E\,, \tag{5}$$

giving that we have started out, our derivation, based on just one molecule solely, before we achieved, the subsequent averaging.

Now, exploring a *likely relationship* between the *classical laws of ideal gases* and *quantum mechanics,* thus supposing discrete energy levels for each individual molecule *(no matter how large may be the related principal quantum numbers that would come into play, in the classical limit),* one may ask the following question:

- *Could Eq. (3) be the basis to build a bridge between "thermodynamics", mainly characterized by the Boltzmann constant, and "quantum mechanics", thereby, basically the energy quantity* $\overline{E}$*, obtained as the averaged value of the discrete energy states of all molecules?*

More specifically, the question is:

- *Can Eq. (3) be the basis to build a bridge between the Boltzmann Constant k and the Planck constant h?*

Here though, while the equality $pV = kT$ points to the law of gases, the next equality $kT = (2/3)\overline{E}$ of Eq.(5), is *no more than a definition* of the *temperature* in terms of the *average translational energy* $\overline{E}$ of the molecules, once k is defined via Eq.(2).

So, $kT = (2/3)\overline{E}$, does not in any way provide us with any relationship between k and h.

In other terms, $\overline{E}$ is to be expected to involve the Planck Constant. Yet this, does not allow us to coin a relationship between h and k, based on Eq.(5), and hence with this latter equation we are bound to fail to establish a relationship between macroscopic properties of an ideal gas and the quantum mechanical description of its constituents.

Thereby we find out that, when we propose to draw any *possible bridge* between the *phenomenological laws of gases* and *quantum mechanics,* we should not really look for a relationship between h and k. Any such effort will be dissolved through a *plain definition of the classical temperature quantity,* in terms of the average translational energy of the molecules, and nothing beyond. However, we can still go ahead to check whether the *phenomenological laws of gases* do match with quantum mechanics, if we could ever explore those laws of gases, which though, do not involve the constant *R* or *k*. That is the key point of our approach.

CONSTANCY OF PV $^{\gamma}$ FOR AN ADIABATICMTRANSFORMATION: QUANTUM APPROACH

There is, in effect, a relationship satisfying the criteria we have just set; this is the one describing an *adiabatic transformation of gases,* in a wide temperature range, *i.e.*

$$PV^{\gamma} = Constant\,, \tag{6}$$

obtained in the familiar way based on the laws of gases, considered together with the first law of thermodynamics [Sommerfeld, 1964], along with the usual definition

$$\gamma = C_P / C_V \,. \tag{7}$$

Here C_V is the *heat to be delivered to one mole of ideal gas at constant volume to increase its temperature as much as 1* ^{o} *K,* and C_P is the *heat to be delivered to one mole of ideal gas at constant pressure to increase its temperature, still as much as 1* ^{o} *K.*

For an ideal gas the internal energy levels of molecules are not excited by definition. In such a case [Van Wylen & Sonntag, 1985], we have

$$C_V = 3R/2\,,\; C_P = 5R/2\,, \tag{8), (9}$$

and the constant γ in Eq. (7) turns to be equal to

$$\gamma = 5/3\,. \tag{10}$$

Hence Eq. (6) acquires the form

$$PV^{5/3} = Constant\,. \tag{11}$$

Any reader in the field, knows that the derivation of this latter relationship is presented in any related text book.

Let us though, for the inquisitive reader right away specify that, the latter relationship, may not be valid for an *irreversible transformation.* The reason is that, through this entire article, we propose to deal with

i) well established states of the gas at hand *(thus excluding any transitory regime, and chiefly, any turbulence),*

ii) a gas, made of strictly *non-interacting constituents,* whereas an *irreversible transformation,* may embody both a *turbulence* and *interactions* between the constituents of the gas.

Anyway [Haar & Wergeland, 1960] suggested a different derivation of Eq. (11), based on the fact that the single-particle energy *E* of a mono-atomic, non-relativistic, diluted gas is proportional to $V^{-2/3}$, *i.e.*

$$E \sim V^{-2/3}\,. \tag{12}$$

To show this, Haar & Wergeland write the energy of a single particle in the i^{th} atom as $\varepsilon_i = V^{-2/3} \cdot f_i$, where f_i is some function of quantum numbers and particle mass for the i^{th} particle. Involving the adiabatic theorem of quantum mechanics *(which implies the constancy of* f_i *under slow variation of the volume),* they straightforwardly arrive at Eq. (12).

Further on Haar & Wergeland noticed that the internal energy of one mole of gas can be written in the form

$$\bar{E} = N_A E\,. \tag{13}$$

Combining Eqs. (12) and (13), one obtains:

$$\bar{E} V^{2/3} = Constant\,. \tag{14}$$

One can additionally write, as usual [cf. Eq. (1)],

$$PV = RT\,, \tag{15}$$

and via Eq. (4), we further derive

$$\bar{E} = \frac{3}{2} PV\,. \tag{16}$$

If now, we multiply the two sides of this latter equation by $V^{2/3}$, and use the *constancy* delineated by Eq. (14), we arrive at

$$PV^{5/3} = Constant\,, \tag{17}$$

which is Eq.(6), written for the ideal gas.

One should mention that just like Eq.(6), provided in all related text books; Eq. (17) too, obtained by Haar & Wergeland, do not tell us, what the affirmed *"adiabatic constant"* specifically is. Moreover, to the moment nobody seems to have even asked what may be the particular *alphanumeric expression* of this constant, if any.

Our goal thus becomes to derive specifically an expression for this *"adiabatic constant",* which - it is worth to stress, still remains *classically unknown* **-** by means of a quantum mechanical description of the ideal gas, well applied to the *"semi-classical limit".* This implies that a principal quantum number for any given molecule can be very large, but this does not create any conceptual difficulties. At the same time, it is important that, in this limit we can use the standard *classical phenomenological laws,* for the ideal gas without any limitations.

In our further approach, as emphasized, it is essential that the ideal gas, is made of strictly *non-interacting molecules,* each behaving as a *simple quantum mechanical particle* locked up *(potential energy – wise)* in an infinitely high box. The wave functions of such non-interacting molecules are not mixed, and thus the internal energy of the ideal gas can be found as a simple sum of eigenvalues of energy for each molecule. Besides, along with the kinetic theory of gases to be valid in the classical limit, we well assume that the *Boyle Mariotte law* [(Eq.(1)] holds for even a single molecule. That is if *R* is replaced by the Boltzmann constant k, in these equations, then one lands at $c_v = (3/2)k$, $c_p = (5/2)k$, defined for just one molecule. This means we can confidently use the ratio C_p/C_v or the same, the ratio c_p/c_v in the quantum world. It means, in particular, that the expression (10) is well applicable to the one molecule at hand, that is, to a single particle confined in a box.

The case of a *photon gas* will be handled separately.

Let us thus consider a particle of mass m at a fixed internal energy state located in a macroscopic *cube* of side L, though without loss of generality. Herein we will consider the non-relativistic case. Our approach anyway can be extended to the relativistic case with no difficulty. The non-relativistic Schrödinger equation furnishes the energy E_n of the particle in the box at a given energy level, *i.e.*

$$E_n = \frac{h^2}{8m}\left(\frac{n_x^{\,2}}{L^2} + \frac{n_y^{\,2}}{L^2} + \frac{n_z^{\,2}}{L^2}\right) = \frac{h^2\left(n_x^{\,2} + n_y^{\,2} + n_z^{\,2}\right)}{8mL^2}, \qquad (18)$$

where n_x, n_y, n_z are the quantum numbers to be associated with the corresponding wave function dependencies on the respective directions x, y and z. For brevity, we introduced the subscript "n" which denotes the specific state characterized by the set of integer numbers n_x, n_y and n_z.

For an ideal gas the *"potential energy"* within the box is zero. Thus, we have

$$E_n = \frac{mv_n^2}{2}, \qquad (19)$$

v_n being the velocity of the particle at the n^{th} energy level.

At the given energy level, the pressure p_n exerted by just one particle on either wall, becomes [cf. Eqs. (3) and (5)]

$$p_n = \frac{mv_n^2}{3L^3} = \frac{2}{3}\frac{E_n}{L^3}. \qquad (20)$$

Now let us calculate *(for just one particle)* the product $p_n V^{5/3}$:

$$p_n V^{5/3} = \frac{2}{3}\,\frac{\dfrac{h^2\left(n_x^{\,2} + n_y^{\,2} + n_z^{\,2}\right)}{8mL^2}}{L^3}\left(L^3\right)^{5/3}. \qquad (21)$$
$$= \frac{h^2\left(n_x^{\,2} + n_y^{\,2} + n_z^{\,2}\right)}{12m}$$

Hence this quantity indeed turns out to be a constant for a given particle of mass m at the given energy level, characterized by the *principal quantum numbers* n_x, n_y and n_z.

Recall that the total energy E_n of Eq. (18) ultimately determines the *quantized velocity* v_n of Eq. (19).

When it is question of many particles instead of just one, normally we would have particles, in general, at different quantized states. This means that, we deal with some energy distribution of molecules at the given temperature, instead of a fixed eigenvalue furnished by Eq. (18), which we derived for a gas consisting of just a single molecule.

In order to describe the *distribution of energy over the molecules* within an elaborated quantum mechanical approach, we have to abandon the strict ideal gas approximation, and add into the Schrödinger equation coming into play, an appropriate potential energy term responsible of the weak interaction of molecules, which will randomly affect all of the molecules of gas at each fixed temperature. We have to stress that such a distribution of *perturbational energy* is to be compatible with the *Maxwellian distribution of velocities.* However, the analysis of this problem falls outside the scope of the present paper. For our immediate purpose**,** it is sufficient to take into consideration an *"average molecule"* at the given temperature T. We can, as conveyed, well visualize the average molecule as a single particle, obeying Eq. (21), thus situated at the *nth* level, and of course associate the given temperature with this energy, along with Eq. (4).

Not to complicate things, let us get focused on the *average particle,* and simply suppose that all others behave the same. Furthermore, all three components of the average velocity at equilibrium are expected to be the same. Thus, we can rewrite Eq. (21) for the macroscopic pressure P_n exerted at the given *average state n* by *one mole* of gas on the walls of the container, as

$$P_n V^{\gamma} = N_A \frac{h^2 n^2}{4m}. \qquad (22)$$

Rigorously speaking, one must write

$$P_n V^{\gamma} = \sum_{i=1}^{N_A} \frac{h^2\left(n_{ix}^{\,2} + n_{iy}^{\,2} + n_{iz}^{\,2}\right)}{12m} = N_A \frac{h^2\,\overline{n^2}}{4m}, \qquad (23)$$

along with the definition

$$\frac{1}{3N_A}\sum_{i=1}^{N_A}\left(n_{ix}^{\,2} + n_{iy}^{\,2} + n_{iz}^{\,2}\right) = \overline{n^2}. \qquad (24)$$

Thus it becomes clear that, if all particles bared the same set of quantum numbers, each with equal quantum numbers along all three directions, *i.e.* $n_x = n_y = n_z = n$, then for the *average molecule,* we can write $n = \sqrt{\overline{n^2}}$.

Eq. (22) does indeed disclose the *Constant* involved by Eq. (6). Note that at the average state *n (i.e. at the given temperature),* the mean square speed of the gas molecules is v_n^2. The average energy is furnished accordingly, via the framework of Eq.(19). Let us calculate what would n be, for 1 mole of, say, O_2, delineating the pressure of 10^5 Pascal *(1 atmosphere),* in a volume of 1 m^3. From Eq. (22) we obtain:

$$n \cong \sqrt{\frac{10^5 \times 4 \times 32 \times 1839 \times 0.9 \cdot 10^{-30}}{6.023 \times 10^{23} \times 6.62^2 \times 10^{-68}}} \approx 28 \text{x} 10^{10}, \qquad (25)$$

which well seems to be a reasonable number, meaning a number fitting our conception of daily phenomena.

Note indeed that this number is well below the Avogadro number N_A *(it is in fact even smaller than the square root of* N_A*),* endorsing well our assumption that the gas molecules do not interact with each other.

Thus finally, our result indicates that the behavior of an ideal gas is nothing, but a *macroscopic manifestation of quantum mechanics.* In particular, the *constancy* of PV^{γ} happens to be rooted to quantum mechanics, and seems to be deep. It is that the quantity *"mass × PV^{γ}"* turns out to be a *Lorentz scalar.*
Thereby, we expect this scalar to be somehow nailed to a *Lorentz invariant universal constant;* this constant, more specifically, turns out to be the *square of the Planck constant.* Accordingly, for a given mass *m,* the quantity PV^{γ} relates to h^2/m; this is what we have revealed in this paper.

Henceforth:

- *The constancy of* PV^{γ} *appears to be an extension of quantum mechanics to macroscopic scales.*

But even more essentially [Yarman 2004 a & b; Yarman 2009; Yarman 2007; Yarman 2010]:

- *It delineates how the internal dynamics displayed by a gas consisting of quantum mechanical particles made of a given mass, is organized in conjunction with the size of the container, the dynamics in question takes place in, and this universally, at all scales.*

Here unfortunately, we have no room to go in any further details of this fundamental problem.

We should like to note that, Eq.(6) is not a *relativistic equation*. That is, if ever the constituents of the gas move at speeds, which cannot be neglected as compared to the speed of light, then it is not a valid relationship, and it should be replaced**,** as insinuated along with Eqs. (21) and (22), by

$$\left(\gamma mc^2\right) PV^{\gamma} = Constant, \qquad (26)$$

where γ is the Lorentz factor, and γm then is the relativistic mass of the average particle.

Note further that the above relationship well holds for a *photon gas,* and we spare the discussion of all of the interesting points, relatedly coming up, for a future work.

CONCLUSION

In this article we aimed to bridge *classical thermodynamics* and *quantum mechanics.* Though we have determined that toward that aim**,** it is in vain to look for a relationship between the Boltzmann constant *k* and the Planck constant *h.* Indeed, a relationship involving both *k* and *h*, such as Eq.(5), is nothing more than a definition of, say, the temperature *(if we choose to go from energy to temperature),* in terms of the translational energy of the particle in hand *[see the discussion we provided below Eq.(5)].* Thus we have picked up on purpose, the relationship $PV^{5/3} = Constant$ to work with, because it constitutes distinctively a closed form of basic gas relationships, which does not involve the Boltzmann constant.

To avoid possible confusions, let us stress that, our goal was not of course, to show that $PV^{5/3}$ remains *constant* through an adiabatic transformation; this is a well known classical relationship. Our goal, was *to calculate specifically, the particular constant, coming into play,* which remained obscure up to now.

In the present contribution we have solved this problem based on quantum mechanics, applied in the semi-classical limit, thus establishing a new link between classical thermodynamics and quantum mechanics in the description of an ideal gas.

The particular value of the constancy of PV^{γ} is something totally missed over almost a century in the literature. The whole thing, in fact, is rooted to an intuition, the first author had developed elsewhere [Yarman 2004 a & b; Yarman 2009; Yarman 2007; Yarman 2010]. In other terms, the constancy of PV^{γ} *(and, likewise, the frame drawn by the law of gases)* seems to be deep, in relation to the fact that the quantity *"mass × PV^{γ}"* turns out to be a *Lorentz scalar,* to cope with the Lorentz transformations on *mass, pressure* and *volume,* that would come into play, were the gas on the whole *(thus, together with its container),* brought to a uniform translational motion.

The Lorentz invariance of *"mass × PV^{γ}"* we came to discover, must further be in a harmony with quantum mechanics; in effect this latter discipline, briefly speaking, based on the *relativistic law of energy conservation,* and *de Broglie relationship,* can be shown to draw a natural symbiosis with the *Special Theory of Relativity,* delineating a *Universal Matter Architecture* [Yarman 2004 a & b; Yarman 2009; Yarman 2007; Yarman 2010], which precisely shapes interrelations, each nailed to the square of the Planck Constant *[cf.*

Eq.(23)], thus, amongst other things, the frame of the relationship *mass* $\times$ PV^{γ} *=Constant,* as we have disclosed herein.

Our approach furthermore, promises the formulation of a thermodynamics, along with just the pair *[Energy, Planck Constant],* instead of the pair [*Temperature, Boltzmann Constant],* this latter pair, aside, embodying the *energy* quantity. In any case, the elimination of the *temperature* quantity, from quantitative descriptions, would, most likely, resolve the present dichotomy between *energy* and *temperature,* more precisely between Planck Constant and Boltzmann Constant.

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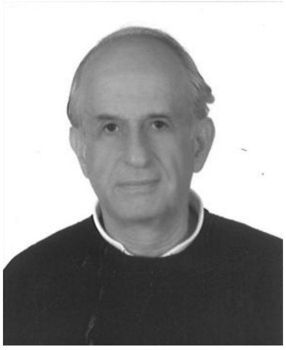
Tolga Yarman

Graduated from Institut National des Sciences Appliquées de Lyon, France (1967), with an M.Sc. in Chemical Engineering, then from the Institute of Nuclear Energy, Technical University of Istanbul (TUI), Turkey (1968), with an M.Sc. in Nuclear Engineering, and then from Massachusetts Institute of Technology (MIT), USA, with a Ph.D. in Nuclear Engineering (1972). Appointed as an Associate Professor on Nuclear Sciences at the Institute of Nuclear Energy, TUI, in 1977, where he became a Full Professor in 1982.

Being awarded by the Council for International Exchange of Scholars, Washington, D.C., enrolled as a Visiting Professor, Engineering Science Department, California Institute of Technology, in 1984. Taught several courses in physical chemistry, atomistic, nuclear engineering & science, energy engineering, thermodynamics, fundamentals of physics, nuclear physics, and quantum mechanics. He also taught courses on nuclear arms race, defense industry, advanced technology, and technology transfer, at the Armed Forces Academy, in Istanbul. Directed many M.Sc. and Ph.D. theses. Author or co-author of several publications made in national and international journals, as well as numerous papers delivered to national and international seminars and conferences. Author of numerous books on energy, nuclear energy, nuclear reactor theory, relativity & quantum mechanics, nuclear arms race and defense strategies, also a book on ethics. Actually enrolled as a faculty member, in T.C. Okan Universitesi, Istanbul, Turkey.

Alexander Kholmetskii

Alexander Kholmetskii was born in 1956 in Novokuznetsk *(Kemerovo region, Siberia, Soviet Union).* In 1979. He graduated from Moscow Engineering & Physical Institute *(MEPHI, Moscow).* In 1986 he got his Ph.D. degree from Belarusian State University *(Minsk)* in the area of experimental nuclear physics. In 1992 he got his Doctor of Sciences degree, still from Belarusian State University in the area of *Mössbauer spectroscopy.* He is a Professor of Physics and Principal Researcher of the Department of Physics of Belarus State University since 1993. Last decade he focused his attention to problems of relativistic physics, including classical electrodynamics and relativistic quantum mechanics. He has made more than two hundred forty scientific publications, including one book, and forty two patents, endorsed by of the Republic of Belarus. In 2007, he got the award of the President of the Republic of Belarus for contribution to the national science.



Önder Korfalı

Graduated from the Mechanical Engineering Faculty of Technical University of Istanbul in 1969, with an M.Sc. degree, and later from Brown University in 1974 with a Ph.D. degree in Mechanical Engineering. Served as Instructor at the Mechanical Engineering Faculty of Middle East Technical University in 1975. Then joining the private sector, worked at managerial level positions for several prominent Turkish companies over a period of twenty five years. Since 1995 being a faculty member of the Engineering and Technology Faculty of Galatasaray University, taught several courses, amongst others, Thermodynamics, Fluid Dynamics, Heat Transfer, Introduction to Aerodynamic Theory, Mechanics, Strength of Materials and Elements of Machinery. Author of very many papers published in international journals, or submitted to international conferences. Member of Sigma Xi.