The Enigma of the Mass.

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Abstract.

The different manifestations of the mass effects in the microphysics (isotope effect) are presented for the first time. The bright effects observe in all branches of physics: nuclear, atomic, and molecular as well as solid state physics. Charge symmetry breaking in the strong interaction occurs because of the difference between the masses of the up and down quarks. At present the Standard Model can’t explain the observed mass pattern (\(M_n\), \(M_p\), \(m_u\), \(m_d\) etc.) and their hierarchy. The last one doesn’t permit us to find the origin of the isotope effect. The origin of the mass of the matter will be clarified when the mechanism of chiral symmetry breaking in QCD is established.

Mass is one of the fundamental properties of matter. It relates to classical as well as modern physics (quantum mechanics or modern theory of gravitation (see, e.g. [1]). Although the physical meaning of mass was discovered by Einstein more than a century ago, when he introduced in physics the concept of rest energy (\(E_0\)) [2], the concept of mass still doesn’t have strict mathematical determination. Indeed, according to the notion of the relativistic physics (see, e.g. [3]) mass is determined by the next expression

\[
m^2 = E^2 - \frac{p^2}{c^2} \tag{1}
\]

And in the case of resting body (\(\vec{p} = 0\)) we have

\[
m = \frac{E_0}{c^2} \tag{2}
\]

From equation (2) it can be seen that the mass is proportioned to the rest energy. If we put \(c = 1\), in that case we see that the mass of body equals its rest energy. The mass of a body is not a constant, it varies with changes in its energy. Namely, rest energy "slumbering" in massive bodies partly is released in chemical and especially nuclear reactions. In spite of equivalence of the mass of the body and rest energy, especially nuclear physics and physics of elementary particles, the task of mass has not been solved. Until present time the spectrum of the discrete hierarchy of elementary particles mass hasn’t had a successful theoretical explanation [4,6]. As is well-known on the boundary of the 19 and 20 centuries there was an opinion that the mass of the electron has the electromagnetic origin [1,4]. However, later investigations showed that the electromagnetic part of the mass of the electron has a small contribution to its full mass [3]. Nevertheless, the modern view connects the origin of the mass with nonlocal gravitational fields, which nature is due to electromagnetic interaction [8 -11].This conclusion reflects those fact, that the space between separated particles in essence isn’t empty, it is filled with the material medium - the physical fields. The space inside the atom is filled with electromagnetic field,
and inside nucleus - more densier and stronger field which is called sometimes meson one.

The present letter is devoted to the elucidation of the origin of mass, so far as only its nature closely connected with the origin of the isotope effect, the experimental manifestation of which more persuasively testified in the last fifty years in all branches of physics (nuclear, atomic, molecular as well as solid state (see, e.g. reviews [12-14])). On the other hand it is necessary to underline that only isotope effect is a direct manifestation of the mass effect in microphysics. It should be added that the direct measurements of the energy of zero-point vibrations owing to isotope effect in solids shows the good agreement of the experimental values with the results of the calculation of quantum electrodynamics in solids [13, 14].

Below we describe shortly the manifestations of the isotope effect in molecular as well as solid state physics (more details see [14]). The discovery [15] of the new fullerene allotropes of carbon, exemplified by C₆₀ and soon followed by an efficient method for their synthesis [14], led to a burst of theoretical and experimental activity on their physical properties. Much of this activity concentrated on the vibrational properties of C₆₀ and their elucidation by Raman scattering [15]. Comparison between theory and experiment was greatly simplified by the high symmetry (Iₖₐₐ₅), resulting in only ten Raman active modes for the isolated molecule and the relative weakness of solid state effect [15], causing the crystalline C₆₀ (c - C₆₀) Raman spectrum at low resolution to deviate only slightly from that expected for the isolated molecule [15]. Since the natural abundance of ¹³C is 1.11% (see, e.g. [12]), almost half of all C₆₀ molecules made from natural graphite contain one or more ¹³C isotopes. If the squared frequency of a vibrational mode in a C₆₀ molecule with n¹³C atoms is written as a series

\[ \omega^2 = \omega^2(0) + \omega^2(1) + \omega^2(2) + \omega^2(3) + \ldots \]

in the mass perturbation (where \( \omega(0) \) is an eigenmode frequency in a C₆₀ molecule with 60 ¹²C atoms), nondegenerate perturbation theory predicts for the two totally symmetric Aₐ modes a first-order correction given

\[ \frac{\omega^2(1)}{\omega^2(0)} = - \frac{n_{13}}{2} . \]  

(3)

This remarkable result, independent of the relative position of the isotopes within the molecule and equally independent of the unperturbed eigenvector, is a direct consequence of the equivalence of all carbon atoms in icosahedral C₆₀. To the same order of accuracy within nondegenerate perturbation theory, the Raman polarizability derivatives corresponding to the perturbed modes are equal to their unperturbed counterparts, since the mode eigenvectors remain unchanged. These results lead to the following conclusion [15]: The Aₐ Raman spectrum from a set of noninteracting C₆₀ molecules will mimic their mass spectrum if the isotope effect on these vibrations can be described in terms of first-order nondegenerate perturbation theory. It is no means obvious that C₆₀ will meet the requirements for the validity of this simple theorem. A nondegenerate perturbation expansion is only valid if the Aₐ mode is sufficiently isolated in frequency from its neighboring modes. Such isolation is not, of course, required by symmetry. Even if a perturbation expansion converges, there is no a priori
reason why second - and higher - order correction to Eq. (3) should be negligible. As was shown in cited paper the experimental Raman spectrum (see below) of $C_{60}$ does agree with the prediction of Eq. (3). Moreover, as was shown in quoted paper, experiments with isotopically enriched samples display the striking correlation between mass and Raman spectra predicted by the above simple theorem. Fig. 1 shows a high - resolution Raman spectrum at 30 K in an energy range close to the high - energy pentagonal - pinch $A_g(2)$ vibration according to [15]. Three peaks are resolved, with integrated intensity of 1.00; 0.95; and 0.35 relative to the strongest peak. The insert of this figure shows the evolution of this spectrum as the sample is heated. The peaks cannot be resolved beyond the melting temperature of CS$_2$ at 150 K. The theoretical fit yields a separation of $0.98 \pm 0.01 \text{ cm}^{-1}$ between two main peaks and $1.02 \pm 0.02 \text{ cm}^{-1}$ between the second and third peaks. The fit also yields full widths at half maximum (FDWHM) of 0.64; 0.70 and 0.90 cm$^{-1}$, respectively. The mass spectrum of this solution shows three strong peaks (Fig. 1$^b$) corresponding to mass numbers 720; 721 and 722, with intensities of 1.00; 0.67 and 0.22 respectively as predicted from the known isotopic abundance of $^{13}$C. The authors [15] assign the highest - energy peak at 1471 cm$^{-1}$ to the $A_g(2)$ mode of isotopically pure $C_{60}$ ($60^{12}$C atoms). The second peak at 1470 cm$^{-1}$ is assigned to $C_{60}$ molecules with one $^{13}$C isotope, and the third peak at 1469 cm$^{-1}$ to $C_{60}$ molecules with two $^{13}$C isotopes. The separation between the peaks is in excellent agreement with the prediction from Eq. (3), which gives $1.02 \text{ cm}^{-1}$. In addition, the width of the Raman peak at 1469 cm$^{-1}$, assigned to a $C_{60}$ molecule with two $^{13}$C atoms, is only 30 % larger than the width of the other peaks. This is consistent with the prediction of Eq. (3) too, that the frequency of the mode will be independent of the relative position of the $^{13}$C isotopes within the molecule. The relative intensity between two isotope and one isotope Raman lines agrees well with the mass spectrum ratios. Concluding this part we stress that the Raman spectra of $C_{60}$ molecules show remarkable correlation with their mass spectra. Thus the study of isotope - related shift offers a sensitive means to probe the vibrational dynamics of $C_{60}$.

Next examples of the dependence of the exciton spectra in solids on the isotope effect demonstrate below. Isotopic substitution only affects the wavefunction of phonons; therefore, the energy values of electron levels in the Schrödinger equation ought to have remained the same. This, however, is not so, since isotopic substitution modifies not only the phonon spectrum, but also the constant of electron-phonon interaction (see [12]). It is for this reason that the energy values of purely electron transition in molecules of hydride and deuteride are found to be different. This effect is even more prominent when we are dealing with a solid [16]. Intercomparison of absorption spectra for thin films of LiH and LiD at room temperature revealed that the longwave maximum (as we know now, the exciton peak ) moves 64.5 meV towards the shorter wavelengths when H is replaced with D [17].

The mirror reflection spectra of mixed and pure LiD crystals cleaved in liquid helium are presented in Fig. 2. For comparison, on the same diagram we have also plotted the reflection spectrum of LiH crystals with clean surface. All
spectra have been measured with the same apparatus under the same conditions. As the deuterium concentration increases, the long-wave maximum broadens and shifts towards the shorter wavelengths. As can clearly be seen in Fig. 2, all spectra exhibit a similar long-wave structure. This circumstance allows us to attribute this structure to the excitation of the ground (1s) and the first excited (2s) exciton states. The energy values of exciton maxima for pure and mixed crystals at 2 K are presented in Table 22 of ref. [12]. The binding energies of excitons $E_b$, calculated by the hydrogen-like formula, and the energies of interband transitions $E_g$ are also given in Table 22.

Going back to Fig. 2, it is hard to miss the growth of $\Delta_{12}$, which in the hydrogen-like model causes an increase of the exciton Rydberg with the replacement of isotopes. When hydrogen is completely replaced with deuterium, the exciton Rydberg (in the Wannier-Mott model) increases by 20% from 40 to 50 meV, whereas $E_g$ exhibits a 2% increase, and at $2 \div 4.2$ K is $\Delta E_g = 103$ meV. This quantity depends on the temperature, and at room temperature is 73 meV, which agrees well enough with $\Delta E_g = 64.5$ meV as found in the paper of Kapustinsky et al. [17]. The single-mode nature of exciton reflection spectra of mixed crystals LiH$_x$D$_{1-x}$ agrees qualitatively with the results obtained with the virtual crystal model (see e.g. Elliott et al. [18]; Onodera and Toyozawa [19]), being at the same time its extreme realization, since the difference between ionization potentials ($\Delta \zeta$) for this compound is zero. According to the virtual crystal model, $\Delta \zeta = 0$ implies that $\Delta E_g = 0$, which is in contradiction with the experimental results for LiH$_x$D$_{1-x}$ crystals. The change in $E_g$ caused by isotopic substitution has been observed for many broad-gap and narrow-gap semiconductor compounds (see also [12]).

All of these results are documented in Table 22 of Ref.[12], where the variation of $E_g$, $E_b$, are shown at the isotope effect. We should highlighted here that the most prominent isotope effect is observed in LiH crystals, where the dependence of $E_b = f (C_H)$ is also observed and investigated. To end this section, let us note that $E_g$ decreases by 97 cm$^{-1}$ when $^7$Li is replaced with $^6$Li.

Detailed investigations of the exciton reflectance spectrum in CdS crystals were done by Zhang et al. [20]. Zhang et al. studied only the effects of Cd substitutions, and were able to explain the observed shifts in the band gap energies, together with the overall temperature dependence of the band gap energies in terms of a two-oscillator model provided that they interpreted the energy shifts of the bound excitons and $n = 1$ polaritons as a function of average S mass reported earlier by Kreingol’d et al. [21] as shifts in the band gap energies. However, Kreingol’d et al. [21] had interpreted these shifts as resulting from isotopic shifts of the free exciton binding energies, and not the band gap energies, based on their observation of different energy shifts of features which they identified as the $n = 2$ free exciton states (for details see [21]). The observations and interpretations, according Meyer et al. [22], presented by Kreingol’d et al. [21] are difficult to understand, since on the one hand a significant band gap shift as a function of the S mass is expected, whereas it is difficult to understand the origin of the relatively huge change in the free exciton binding energies which they claimed. Very recently Meyer et al. [22] reexamine
the optical spectra of CdS as function of average S mass, using samples grown with natural Cd and either natural S (∼95% 32S), or highly enriched (99% 34S). These authors observed shifts of the bound excitons and the n = 1 free exciton edges consistent with those reported by Kreingol’d et al. [21], but, contrary to their results, Meyer et al. observed essentially identical shifts of the free exciton excited states, as seen in both reflection and luminescence spectroscopy. The reflectivity and photoluminescence spectra in polarized light ($\vec{E} \perp \vec{C}$) over the A and B exciton energy regions for the two samples depicted on the Fig. 3. For the $\vec{E} \perp \vec{C}$ polarization used in Fig. 3 both A and B excitons have allowed transitions, and therefore reflectivity signatures. Fig. 3 reveals both reflectivity signatures of the n = 2 and 3 states of the A exciton as well that of the n = 2 state of the B exciton.

In Table 18 of Ref. [14] the results of Meyer et al. summarized the energy differences $\Delta E = E (Cd^{34}S) - E (Cd^{nat}S)$, of a large number of bound exciton and free exciton transitions, measured using photoluminescence, absorption, and reflectivity spectroscopy, in CdS made from natural S (Cd$^{nat}$S, 95% 32S) and from highly isotopically enriched 34S (Cd$^{34}$S, 99% 34S). As we can see from Fig. 3, all of the observed shifts are consistent with a single value, 10.8±0.2 cm$^{-1}$. Several of the donor bound exciton photoluminescence transitions, which in paper [22] can be measured with high accuracy, reveal shifts which differ from each other by more than the relevant uncertainties, although all agree with the 10.8±0.2 cm$^{-1}$ average shift. These small differences in the shift energies for donor bound exciton transitions may reflect a small isotopic dependence of the donor binding energy in CdS (see, also [12]). This value of 10.8±0.2 cm$^{-1}$ shift agrees well with the value of 11.8 cm$^{-1}$ reported early by Kreingol’d et al. [21] for the $B_{n=1}$ transition, particularly when one takes into account the fact that enriched 32S was used in that earlier study, whereas Meyer et al. have used natural S in place of an isotopically enriched Cd$^{32}$S (for details see [22]).

Authors [21] conclude that all of the observed shifts arise predominantly from an isotopic dependence of the band gap energies, and that the contribution from any isotopic dependence of the free exciton binding energies is much smaller. On the basis of the observed temperature dependencies of the excitonic transitions energies, together with a simple two-oscillator model, Zhang et al. [20] earlier calculated such a difference, predicting a shift with the S isotopic mass of 950 μeV/amu for the A exciton and 724 μeV/amu for the B exciton. Reflectivity and photoluminescence study of $nat$Cd$^{32}$S and $nat$Cd$^{34}$S performed by Kreingol’d et al. [21] shows that for anion isotope substitution the ground state (n = 1) energies of both A and B excitons have a positive energy shifts with rate of $\partial E/\partial M_S = 740 \mu eV/amu$. Results of Meyer et al. [22] are consistent with a shift of $\sim 710 \mu eV/amu$ for both A and B excitons. Finally, it is interesting to note that the shift of the exciton energies with Cd mass is 56 μeV/amu [20], an order of magnitude less than found for the S mass (more details see [12, 13]).

The brought examples clearly indicate mass dependence of the electron and phonon states (see more details [14]) but on the other side it simply under-
lines the primary importance in microphysics the difference of mass between neutron ($M_n$) and proton ($M_p$). Really small difference in their masses $M_n - M_p = 1.2333317$ MeV leads to the bright effects in microphysics. According to the last data [9], the experimental neutron-proton mass difference of $M_n - M_p = 1.2333317$ MeV is received as estimated electromagnetic contribution $M_n - M_p \, |^{\text{em}} = -0.76 \pm 0.30$ MeV, and the remaining mass difference is determined to a strong isospin breaking contribution of $M_n - M_p \, |^{d-u} = 2.05 \pm 0.30$ MeV. In other words the last contribution is a result of difference in mass of d- and u-quarks (see, also [10, 11]).

As we all know, the observed world - stars, planets, galaxy as well as surrounding objects consist from the nuclei, neutrons, protons and electrons. The mass of electrons has a small contribution to the total mass (less than 0.1%) (see, e.g. [1]). Therefore, that we knew that the origin of the mass of the observed worlds needs to be elucidated the origin of nuclear mass. As we know the nucleon consists from u- and d- quarks. But the mass of u- and d- quarks is so small, that is their sum is a small part of the nucleon mass (1 - 2 % [6]). In modern physics of elementary particles it is considered that the mass of nucleon arises from the spontaneous breaking of a chiral symmetry in quantum chromodynamics (QCD) [23] and may be expressed over vacuum condensate (see [5] and references therein). This model has an approximate formula which expresses the mass of nucleon over quarks condensate [5]

$$m = \left[-2(2\pi)^2 \langle 0 | \bar{q} q | 0 \rangle\right]^{1/3}$$

where $m$ is nucleon mass, $\langle 0 | \bar{q} q | 0 \rangle$ is quarks condensate, $q$ is the field of u- or d- quarks. The chiral symmetry in QCD result in the expression for the quarks condensate (so called Gell - Mann - Oakes - Renner formula [24])

$$\langle 0 | \bar{q} q | 0 \rangle = \frac{m_m f_\pi}{m_u + m_d}$$

Here $m_\pi$ and $f_\pi$ are the mass and decay constant of $\pi$-meson. The defined value of quarks condensate on the ground of $\tau$-decay [5,6] equals

$$\langle 0 | \bar{q} q | 0 \rangle = -(254 \text{ MeV})^3 \pm 10\%.$$  \hspace{1cm} (6)

Put the last value into the expression (4) it gives the nucleon’s mass $m = 1.08$ GeV, when the experimental value of nucleon’s mass equals $m = 0.94$ MeV. From comparison of these values we see that the difference between experimental value of $m$ and theoretical estimation is 0.15 GeV, that surpasses the experimental value of the difference $M_n - M_p = 1.2333317$ MeV much order. The last one means that in such model (as well as in the model of constituent quarks) we have neither the mass difference of the nucleons nor its number in nuclei and, consequently, isotope effect. But the experimental manifestations of the isotope effect was demonstrated above in the different branches of microphysics. Considering the quarks structure of nucleon (the wavefunction of the neutron is udd, and for proton one is uud) that is the quark structure indicates the different construction of the neutron and proton, but this model doesn’t quantitative describe the mass of nucleons.

Thus, the origin of the isotope effect is closely connected with the different origin of u- and d- quarks and with solution the spectrum and hierarchy of the elementary particles mass and more common with the solution of the nature of mass (see, also [25]).
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Figure captions.

Fig. 1. a - unpolarized Raman spectrum in the frequency region of the pentagonal - pinch mode, for a frozen sample of nonisotopically enriched C\textsubscript{60} in CS\textsubscript{2} at 30 K. The points are the experimental data, and the solid curve is a three - Lorentzian fit. The highest - frequency peak is assigned to the totally symmetric pentagonal - pinch A\textsubscript{g} mode in isotopically pure \textsuperscript{12}C\textsubscript{60}. The other two peaks are assigned to the perturbed pentagonal - pinch mode in molecules having one and two \textsuperscript{13}C - enriched C\textsubscript{60}, respectively. The insert shows the evolution of these peaks as the solution is heated. b - the points give the measured unpolarized raman spectrum in the pentagonal - pinch region for a frozen solution of \textsuperscript{13}C - enriched C\textsubscript{60} in CS\textsubscript{2} at 30 K. The solid line is a theoretical spectrum computed using the sample’s mass spectrum, as described in the text (after [15]).

Fig. 2. Mirror reflection spectra of crystals: 1 - LiH; 2 - LiH\textsubscript{x}D\textsubscript{1-x}; 3 - LiD; at 4.2 K. 4 - source of light without crystal. Spectral resolution of the instrument is indicated on the diagram (after [12]).

Fig. 3. a - Reflection spectra in the A and B excitonic polaritons region of Cd\textsuperscript{nat}S and Cd\textsuperscript{34}S at 1.3K with incident light in the $\vec{E} \perp \vec{C}$. The broken vertical lines connecting peaks indicate measured energy shifts reported in Table 18 of Ref. [14]. In this polarization, the n = 2 and 3 excited states of the A exciton, and the n = 2 excited state of the B exciton, can be observed. b - Polarized photoluminescence spectra in the region of the A\textsubscript{n} = 2 and A\textsubscript{n} = 3 free exciton recombination lines of Cd\textsuperscript{nat}S and Cd\textsuperscript{34}S taken at 1.3 K with the $\vec{E} \perp \vec{C}$. The broken vertical lines connecting peaks indicate measured energy shifts reported in Table 18 of Ref. [14] (after [22]).

References.

1. M. Jammer, Concepts of mass in classical and modern physics, Harvard University Press, Cambridge - Massachsets (1961).
2. A. Einstein, Ann. Phys. (Leipzig) 20, 371 (1906).
3. L.D. Landau, E.M. Lifshitz, The classical theory of fields, Pergamon, New York (1958).
4. L.B. Okun, Physics Today, June 1989; Uspekhi Fiz. Nauk 158, 512 (1989) (in Russian).
5. B.L. Ioffe, Uspekhi Fiz. Nauk 171, 1273 (2001) (in Russian); Progr. Part. Nucl. Phys. 56, 232 (2006).
6. C.D. Frogatt, Surveys High Energy Physics 18, 77 (2003); The Problem of Mass, ArX:hep - ph/0312220.
7. A. Dobado and A.L. Maroto, Phys. Rev. D60, 104045-9 (1999).
8. J.J. Kelly, Phys. Rev. C70, 068202 (2004).
9. S.R. Beane, K. Originas and M.J. Savage, Nucl. Phys. B768, 38, (2007).
10. G.A. Miller, A.K. Opper, E.J. Stephenson, Annual Review of Nuclear Science 56, 253 (2006).
11. G.A. Miller, Phys. Rev. Lett. 99, 112001 (2007); The Neutron Negative Central Charge Density: an Inclusive - Exclusive Connection, ArXiv 0806.3977.
12. V.G. Plekhanov, Phys. Reports 410, 1 (2005).
13. M. Cardona, M.L.W. Thewalt, Rev. Mod. Phys. 77, 1173 (2005).
14. V.G. Plekhanov, will be published.
15. J. Menendez and J.B. Page, Vibrational spectroscopy of C_{60}, in, M. Cardona and G. Guntherodt, eds., Light Scattering in Solids VIII, Springer, Berlin - Heidelberg (2000) (Vol. 76 in Topics in Applied Physics).
16. V.G. Plekhanov, Isotope effects in solid state physics, Academic Press, San Diego (2001).
17. A.F. Kapustinsky, L.M. Shamovsky, K.S. Bayushkina, Acta Physicochim. (USSR) 7, 799 (1937).
18. R.J. Elliott, J.AA. Krumhansl, P.L. Leath, Rev. Mod. Phys. 46, 465 (1974).
19. Y. Onodera and Y. Toyozawa, J. Phys. Soc. Japan 24, 341 (1968).
20. M. Zhang, M. Ghieler, T. Ruf, Phys. Rev. B57, 9716 (1998).
21. F.I. Kreingol’d, K.F. Lider, M.B. Shabaeva, Fiz. Tverd. Tela 26, 3940 (1984) (in Russian).
22. T.A. Meyer, M.L.W. Thewalt and R. Lauck, Phys. Rev. B69, 115214-5 (2004).
23. J. Grasser and H. Leutwyller, Phys. Reports 87, 77 (1982); H. Leutwyller, Insights and Puzzles in Light Quark Physics, ZrXiv:hep - ph/070063138.
24. M. Gell-Mann, R.J. Oakes, B. Renner, Phys. Rev. 175, 2195 (1968).
25. I. F. Ginzburg, Uspekhi Fiz. Nauk (Moscow) 179, 525 (2009) (in Russian).