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Analytic Solutions for Equilibrium Configuration of General Relativistic Gas Spheres II

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Two new analytic solutions of Einstein field equations for a static and spherical distribution of perfect fluid are obtained. One of them describes successfully the structure of a massive neutron star. For example, the mass, the radius and the central density are estimated to be $1.11M_{\odot}$, 4.64km and 10^{16} g/cm^3, respectively. While the other corresponds to a less massive star with $0.757M_{\odot}$, 7.3km and 10^{15}g/cm^3.

§ 1. Introduction

The need for going beyond the framework of Newtonian gravitational theory has been recognized in two types of systems: the Universe as a whole (cosmology); and a highly collapsed isolated bodies (neutron stars, black holes). Whereas various analytic solutions of Einstein field equations have been obtained in order to deal with a matter of comsology, only a few analytic solutions suitable for dense stars have been so far proposed[1].

Usually, the equilibrium configuration of neutron stars has been investigated by numerical method[2]. Although numerical solutions have the advantage of physical exactitude, especially on the equation of state, they are quite inappropriate to an analytic investigation.

Very recently, from this point of view, Kuchowicz[3] and the present authors[4]* proposed independently a new analytic solution for the gravitational equilibrium of perfect fluid. (Hereafter we refer to this solution as "Sol. I".) In the present paper we newly propose two analytic solutions other than Sol. I for the same problem, which seem considerably suitable to describe the structure of neutron stars.

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*) The following misprints in this reference should be noted: In Eq. (24) the exponent of wave bracket should be 1/2. In line 4 on page 35, replace (8) by (18).

§ 2. Analytic Solutions

The expression for the interval in a static and spherically symmetric field can be written in the following form:

$$ds^2 = e^{\nu}c^2dt^2 - e^{\lambda}dr^2 - r^2d\theta^2 - r^2\sin^2\theta d\varphi^2 \quad , \tag{1}$$

where ν and λ are functions only of the radial space coordinate r.

With use of the energy-momentum tensor for a perfect fluid, Einstein field equations take the form:

$$\varkappa P = e^{-\lambda}\left(\frac{\nu'}{r} + \frac{1}{r^2}\right) - \frac{1}{r^2} \quad , \tag{2}$$

$$\varkappa P = \frac{1}{2}e^{-\lambda}\left(\nu'' + \frac{\nu'^2}{2} - \frac{\nu'\lambda'}{2} + \frac{\nu' - \lambda'}{r}\right) \quad , \tag{3}$$

$$\varkappa \rho c^2 = e^{-\lambda}\left(\frac{\lambda'}{r} - \frac{1}{r^2}\right) + \frac{1}{r^2} \quad , \tag{4}$$

where P and ρ are the pressure and the density of fluid in a proper system, $\varkappa = 8\pi G/c^4$ and the primes denote differentiation with respect to r.

It is easily verified that the following set of Eqs. (5) and (6) satisfy a set of field equations (2) to (4):

$$e^{\nu} = (a + x^2)^3 \quad , \tag{5}$$

$$e^{-\lambda} = 1 - \frac{3}{2}\frac{x^2}{a + x^2}\left\{1 + \frac{B}{(a + 4x^2)^{1/2}}\right\} \quad , \tag{6}$$

where $x = r/R$ and a, B and R are constants.

Substituting them into Eqs. (2) and (4), we can get a following set of expressions for pressure and density:

$$\varkappa R^2 P = \frac{3}{2}\frac{1}{(a + x^2)^2}\left\{3(a - x^2) - B\frac{a + 7x^2}{(a + 4x^2)^{1/2}}\right\} \quad , \tag{7}$$

$$\varkappa R^2 \rho c^2 = \frac{3}{2}\frac{1}{(a + x^2)^2}\left\{(3a + x^2) + 3aB\frac{a + 3x^2}{(a + 4x^2)^{3/2}}\right\} \quad , \tag{8}$$

which is just the equation of state written in a parametric form. The sound velocity v_s in this fluid is derived from Eqs. (7) and (8) as follows:

$$\left(\frac{v_s}{c}\right)^2 = \frac{\partial P}{\partial \rho} = \frac{3(a + 4x^2)\{(3a - x^2)(a + 4x^2)^{3/2} + B(a^2 - ax^2 - 14x^4)\}}{(5a + x^2)(a + 4x^2)^{5/2} + 3aB(5a^2 + 23ax^2 + 30x^4)} \quad . \tag{9}$$

Hereafter we refer to this solution as "Sol. II".

Another solution of field equations can be found out as follows:

$$e^{\nu} = Ae^{u} \tag{10}$$

$$e^{-\lambda} = 1 - [\beta + I_e(1+u)]ue^{-u} \tag{11}$$

where $u = ar^2$ and $I_e(z) = \int_1^z (e^{t-1}/t)dt$ and a, β and A are constants. we give the values of $I_e(z)$ in Table 1.

Table 1. Values of $I_e(z) = \int_1^z (e^{t-1}/t)dt$.

z	0	2	4	6	8
1.000	.000000	.001999	.003998	.005997	.007996
10	.009995	.011994	.013993	.015992	.017991
20	.019990	.021987	.023989	.025988	.027988
30	.029990	.031988	.033988	.035988	.037987
40	.039988	.041989	.043989	.045990	.047992
50	.049993	.051994	.053996	.055997	.058000
60	.060002	.062005	.064007	.066010	.068013
70	.070017	.072020	.074024	.076029	.078033
80	.080038	.082043	.084049	.086054	.088060
90	.090067	.092074	.094081	.096088	.098096
1.100	.100103	.102112	.104121	.106130	.108140
10	.110150	.112160	.114171	.116182	.118194
20	.120206	.122218	.124231	.126244	.128258
30	.130273	.132287	.134302	.136318	.138334
40	.140351	.142368	.144386	.146404	.148422
50	.150442	.152461	.154482	.156502	.158524
60	.160546	.162568	.164591	.166615	.168639
70	.170664	.172689	.174715	.176741	.178768
80	.180796	.182825	.184853	.186883	.188913
90	.190944	.192976	.195008	.197041	.199074

Substitution of them into Eqs. (2) and (4) leads again to the equation of state:

$$\varkappa P \frac{R^2}{a} = 2 - (1+2u)[\beta + I_e(1+u)]e^{-u} , \tag{12}$$

$$\varkappa \rho \frac{R^2}{a} c^2 = (3-2u)[\beta + I_e(1+u)]e^{-u} + \frac{2u}{1+u} . \tag{13}$$

The sound velocity v_s is in the form:

$$\left(\frac{v_s}{c}\right)^2 = \frac{(1+u)^2(1-2u)[\beta + I_e(1+u)]e^{-u} + (1+u)(1+2u)}{(1+u)(5-2u)[\beta + I_e(1+u)]e^{-u} - (5+u-2u^2)} . \tag{14}$$

Hereafter we refer to this solution as "Sol. III".

§ 3. Application to neutron stars

Now we go on to apply the above obtained solutions to describe the structure of the neutron star, determining the values of parameters a, B, β, A and R from the boundary conditions.

3. 1 Application of Sol. II

i) Determination of parameters from boundary conditions

At the center of the star $x=0$, Eqs. (5) to (9) are reduced to the following simple forms:

$$\exp(\nu_c)=a^3, \qquad \exp(\lambda_c)=1 \quad , \tag{15}$$

$$\varkappa R^2 P_c=\frac{3}{2}\frac{1}{a^2}(3a-Ba^{1/2})=\frac{3}{2a}(3-\alpha) \quad , \tag{16}$$

$$\varkappa R^2\rho_c c^2=\frac{3}{2}\frac{1}{a^2}(3a+3a^{1/2}B)=\frac{9}{2a}(1+\alpha) \quad , \tag{17}$$

$$\left(\frac{v_s}{c}\right)_c^2=\frac{3}{5}\frac{3+\alpha}{1+3\alpha} \quad , \tag{18}$$

where the subscript c refers to quantities at the center, and $\alpha=B/a^{1/2}$.

Since $\exp[-\nu/2]$ indicates the gravitational redshift, $\exp[-\nu_c/2]=a^{-3/2}$ must be greater than unity. Then we have $a<1$.

From Eq. (16), we see the value of α should be upward bounded, that is, $\alpha<3$. On the other hand the relativistic causality $v_s\leqq c$ at the center assigns the lower limit of α to 1/3 from Eq. (18). Thus α is restricted to the range

$$1/3\leqq\alpha<3 \quad . \tag{19}$$

The ratio of the pressure and density at the center is given by

$$\frac{P_c}{\rho_c c^2}=\frac{3-\alpha}{3+3\alpha} \quad . \tag{20}$$

The value of this ratio are 2/3 and 1/3 for $\alpha=1/3$ and $\alpha=1$, respectively. Thus this ratio decreases with increasing α. Hence α may be regarded as a measure of softness of the equation of state.

On the surface of the star where $P=0$, we can get the following relation from Eq. (7):

$$\alpha=\frac{3(1-\xi)(1+4\xi)^{1/2}}{(1+7\xi)} \quad , \tag{21}$$

where $\xi = x_b^2/a$ and x_b is the reduced stellar radius. Hereafter the subscript b refers to quantities on the stellar outer boundary. On the surface $r_b = Rx_b$, the line element must connect with the well-known Schwarzschild solution. Thus we have

$$\exp(\nu_b) = \exp(-\lambda_b) = 1 - r_g/r_b \quad , \tag{22}$$

where $r_g = 2GM/c^2$ is the gravitational radius of the sphere with mass M.

Combining Eqs. (5), (6), (21) and (22), we can get

$$a^3 = \frac{1}{(1+\xi)^2(1+7\xi)} \quad , \tag{23}$$

$$\frac{r_g}{r_b} = \frac{6\xi}{1+7\xi} \quad . \tag{24}$$

Once we specify the value of a, we can determine the values of ξ, a, B, r_g, ν_b and λ_b, by making use of Eqs. (21) to (24). These values are shown in Table 2 for the typical cases of $a = 1/3$ and 1.

Table 2. Values of the non-dimentional parameters for $a = 1/3$ and 1.

a	1/3	1
$P_c/\rho_c c^2$	2/3	1/3
ξ	0.670352	0.301716
a	0.397827	0.574525
B	0.210245	0.757974
$\exp[-\nu_c/2]$	3.9853	2.2963
$\exp[-\nu_b/2]$	1.8461	1.5462
r_b/R	0.516415	0.416345
r_g/R	0.364882	0.242193
r_b/r_g	1.4153	1.7191
ρ_b/ρ_g	0.36707	0.49623

The pressure and the density distributions which are normalized at the center are shown in Figures 1 and 2. The arrows denote the boundary of the sphere. It should be noted that both pressure and density decrease monotonically outward though the drop of density is very slight especially for large value of a.

ii) Physical quantities

Using the value of R obtained from Eq. (17) by specifying ρ_c, we can determine the physical quantities such as P_c, r_b, r_g and M. For example, in Table 3 we show them obtained by specifying the typical value of $\rho_c = 1.0 \times 10^{16}$ g/cm^3. These values are essentially in agreement with the results obtained by the numerical calculation by using the theory of nuclear matter.[2),5)]

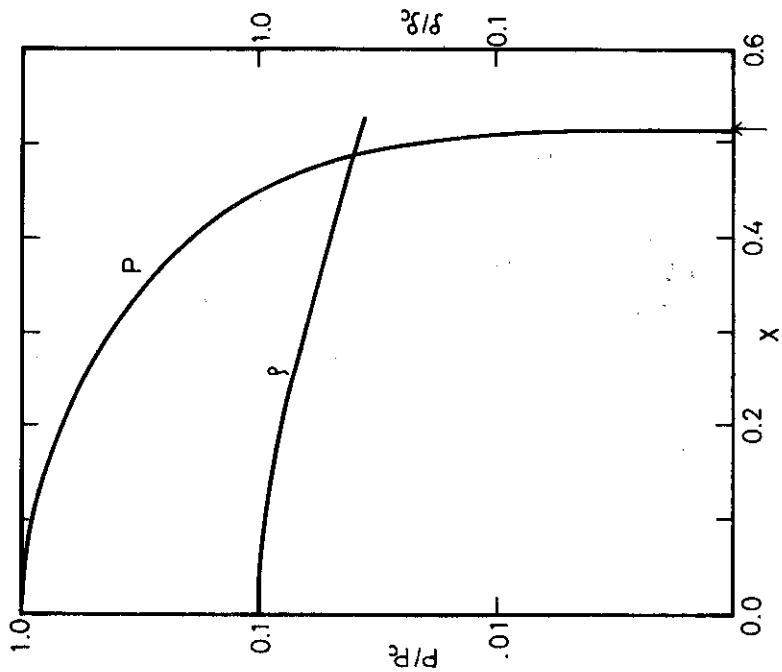

Figure 1. Interior distributions of pressure and density for $\alpha = 1/3$ in Sol. II. Normalizations are made at the center. The arrow denotes the boundary of the sphere.

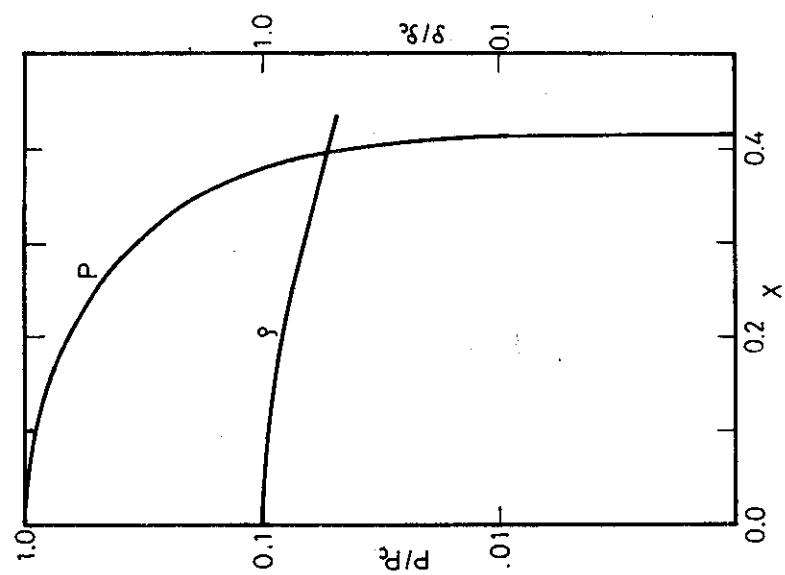

Figure 2. Interior distributions of pressure and density for $\alpha = 1$ in Sol. II.

Table 3. Values of the physical quantities for $a=1/3$ and 1.

a	1/3	1
ρ_c (g/cm^3)	1.0×10^{16}	1.0×10^{16}
P_c (dyne/cm^2)	6.0×10^{36}	3.0×10^{36}
R (km)	8.99	9.17
r_b (km)	4.64	3.82
r_g (km)	3.28	2.22
M ($M_\odot$)	1.11	0.76

3.2 Application of Sol. III

i) Determination of parameters from boundary conditions

At the center $x=0$, Eqs. (10) to (14) are reduced to

$$\exp(\nu_c)=A, \qquad \exp(\lambda_c)=1 \quad , \tag{25}$$

$$\varkappa\frac{R^2}{a}P_c=2-\beta\,, \tag{26}$$

$$\varkappa\rho_c\frac{R^2}{a}c^2=3\beta\,, \tag{27}$$

$$\left(\frac{V_s}{c}\right)_c^2=\frac{\beta+1}{5(\beta-1)} \tag{28}$$

From the first equation in (25), we can get $A<1$, because $\exp[-\nu/2]$ indicates the gravitational redshift.

Both the relativistic causality and the physical condition $P_c>0$ require the restriction for β as follows:

$$3/2\leqq\beta<2\,, \tag{29}$$

which is obtained from Eqs. (28) and (26). The ratio of the central pressure to density is given by

$$\frac{P_c}{\rho_c c^2}=\frac{2-\beta}{3\beta} \quad , \tag{30}$$

the values of which are 1/9 and 1/18 for $\beta=3/2$ and 12/7, respectively. This ratio decreases with increasing β. Hence β may be also regarded as a measure of softness of the equation of state.

On the surface of the star, we can get, from Eqs. (10), (11), (12) and (22), the following relations:

$$2\exp(u_b)=(1+2u_b)[\beta+I_e(1+u_b)] \quad , \tag{31}$$

$$A=\frac{1}{1+2u_b}\exp(-u_b) \quad , \tag{32}$$

$$\frac{r_g}{r_b}=\frac{2u_b}{1+2\,u_b} \quad . \tag{33}$$

Specifying the value of u_b, we can get the values of β, A, $P_c/\rho_c c^2$ and r_b/r_g by using Eqs. (31), (32), (30), (28) and (33). These values are given in Table 4 in the typical case $u_b=0.22$, where the value of β satisfies the condition (29).

Table 4. Values of the mathematical and physical quantities for Sol. III.

u_b	0.22	ρ_c (g/cm^3)	1.0×10^{15}
β	1.509	P_c (dyne/cm^2)	9.7×10^{34}
A	0.557	r_b (km)	7.31
$P_c/\rho_c c^2$	0.108	r_g (km)	2.23
r_b/r_g	3.273	M ($M_\odot$)	0.757

The distributions of pressure and density are shown in Figure 3 in the same way as in Sol. II.

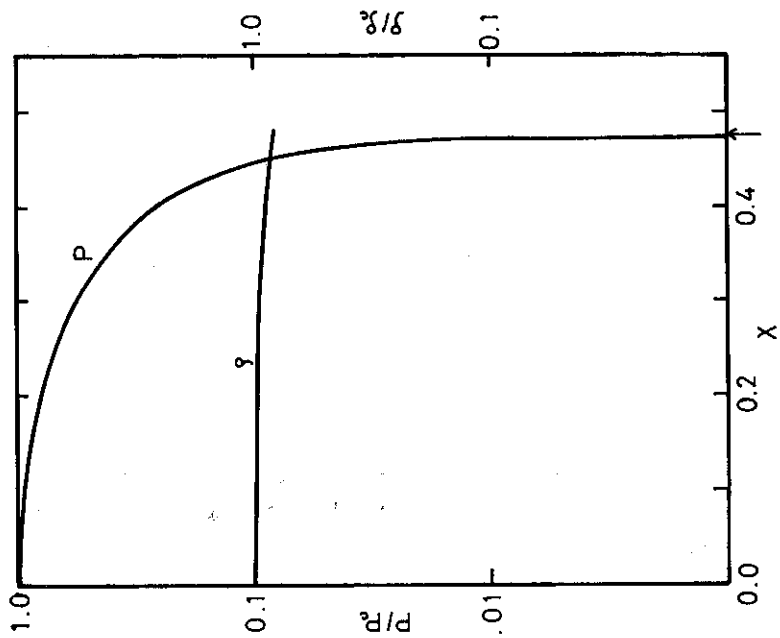

Figure 3. Interior distributions of pressure and density for $\beta=1.509$ in Sol. III.

ii) Physical quantities

Determining the value of R^2/a from Eq. (27), we can get the values of physical quantities $r_b = R(u_b a)^{1/2}$, r_g, M and P_c. These are shown in Table 4 for a fixed value of $\rho_c = 10^{15}\text{g/cm}^3$.

§ 4. Concluding Remarks

In Sol. II, for specified value of $\rho_c = 10^{16}\text{g/cm}^3$, the radii are 4.64km and 3.82km and the gravitational masses are $1.11\text{M}_\odot$ and $0.76\text{M}_\odot$ for $\alpha = 1/3$ and 1, respectively. In Sol. III, for specified value of $\rho_c = 10^{15}\text{g/cm}^3$, the radius is 7.3km and the gravitational mass is $0.757\text{M}_\odot$ for $\beta = 1.509$. From the above obtained results, we may conclude that Sol. II corresponds to the massive neutron star, as in the case of Sol. I, while Sol. III to the less massive star.

References

1) R. C. Tolman, Phys. Rev. **55** (1939), 364.
2) G. Börner, Springer Tracts Mod. Phys. **69** (1973), 1.
K. Kaminisi, Phys. Rep. Kumamoto Univ. **1** (1973), 11.
3) B. Kuchowicz, Astrophys. Space Sci. **33** (1975), L13.
4) K. Arai and K. Kaminisi, Phys. Rep. Kumamoto Univ. **2** (1975), 29.
5) R. C. Malone, M. B. Johnson and H. A. Bethe, Astrophys. J. **199** (1975), 741.

Physics Reports of the Kumamoto University, Vol. 2, No. 2 (1976)

Intensity Distribution of the $^1A_{1g} \rightarrow (^1B_{1u}$ and $^1E_{1u})$ Band Systems of Benzene

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The intensity distribution of the $^1A_{1g} \rightarrow (^1B_{1u}$ and $^1E_{1u})$ band systems is discussed in the view point of A. D. Liehr. The intensity distribution is calculated with the extension of Yu. E. Perlin's method.

The calculation is based on the simple hamiltonian which is adopted by van der Waals et al. Finally the vibronic coupling parameter a is estimated empirically. This estimated value is considerably larger than the evaluated value of M. H. Perrin et al.

§ 1. Introduction

A. D. Liehr argues that the electronic states $^1B_{1u}$ and $^1E_{1u}$ can not be approximated separately by the Born Oppenheimer approximation but that the triple manifold of these states should be taken into consideration[1]. According to his arguments, the simple Herzberg-Teller approximation which is based on the Born Oppenheimer approximation, is unappropriate for the investigation of the absorption band systems $^1A_{1g} \rightarrow (^1B_{1u}$ and $^1E_{1u})$ of benzene. Thus the method of Longuet-Higgins or Liehr-Moffit, are appropriate for the investigation[1)2)]. The latter is devised in connection with the Jahn-Teller effect and the pseudo Jahn-Teller effect. M. H. Perrin et al evaluate the intensity of $^1A_{1g} \rightarrow {}^1B_{1u}$ band system of benzene with this method[3)]. The hamiltonian is similar to the hamiltonian of van der Waals et al[4)]. In this article the present authors extend the method of Yu. E. Perlin and then apply the extended method to the investigation of the $^1A_{1g} \rightarrow (^1B_{1u}$ and $^1E_{1u})$ band systems of benzene[5)].

The calculation is based on the hamiltonian which is similar to one of van der Waals et al.

§ 2. Formulations

The $^1B_{1u}$ and $^1E_{1u}$ electronic states are represented by p and (β,β') as the

previous article[6]. Here the electronic state means the electronic states for some fixed nuclear configuration which is in a form of regular hexagon[2]. β is transformed like $\cos\phi$ under any operation of rotation about the sixfold axis and β'

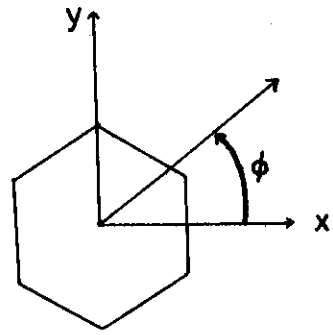


Fig. 1. The coordinate system.

is transformed like $\sin\phi$ under the same operation. The vibrational normal coordinates of the e_{2g}-8th mode, are represented by δQ and $\delta Q'$. δQ is transformed like $\cos 2\phi$ under any operation of rotation about the sixfold axis and $\delta Q'$ is transformed like $\sin 2\phi$ under the same operation. δQ and $\delta Q'$ are normalized as follows;

$$\{(m\omega)/\hbar\}^{1/2}\times(\text{actual displacement}),$$

where ω is the characteristic angular frequency for the e_{2g}-8th mode (e_{2g} strech mode). According to van der Waals et al or M. H. Perrin et al, the hamiltonian for the triple manifold of $^1B_{1u}$ and $^1E_{1u}$ states, is assumed as follows[3)4)];

$$H(p,\beta,\beta') = H_0(p,\beta,\beta') + H_1(p,\beta,\beta'),$$

$$H_0(p,\beta,\beta') = \begin{pmatrix} \hbar\Omega_p^{(0)} + H_n^{(p)} & 0 & 0 \\ 0 & \hbar\Omega_\beta^{(0)} + H_n^{(\beta)} & 0 \\ 0 & 0 & \hbar\Omega_{\beta'}^{(0)} + H_n^{(\beta')} \end{pmatrix}$$

and

$$H_1(p,\beta,\beta') = v\begin{pmatrix} 0 & \delta Q & -\delta Q' \\ \delta Q & 0 & 0 \\ -\delta Q' & 0 & 0 \end{pmatrix},$$

where the first row and the first column refer to the p electronic state. The second row and the second column refer to the β electronic state. The third row and the third column refer to the β' electronic state. $H_n^{(p)}$, $H_n^{(\beta)}$ and $H_n^{(\beta')}$ are the pure vibrational hamiltonians. And then it is assumed that $H_n^{(p)} = H_n^{(\beta)} =$

$H_n^{(\beta')}$. It is evident that $\Omega_\beta^{(0)}=\Omega_\beta^{(0)}$.

Now the intensity distribution of the $^1A_{1g}\rightarrow(^1B_{1u}$ and $^1E_{1u})$ band systems, is expressed except for some frequency factor, as follows[5];

$$I(\Omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\ \exp(i\Omega t)<00Q|<0|\boldsymbol{m}_e\exp\{(-it/\hbar)H(p,\beta,\beta')\}$$
$$\boldsymbol{m}_e\exp\{(it/\hbar)H_n^{(0)}\}|0>|00Q>, \tag{1}$$

where $|0>|00Q>$ represents the ground vibronic state and $\boldsymbol{m}_e$ represents the electronic part of electric dipole moment operator. $H_n^{(0)}$ is the vibrational hamiltonian for the ground electronic state.

The expression (1) is reduced to the following form;

$$I(\Omega)=\frac{1}{\pi}|<0|\boldsymbol{m}_e|\beta'>|^2\int_{-\infty}^{\infty}dt<00Q|\exp\{i(\hbar\Omega-\hbar\Omega_\beta^{(0)}-H_n^{(p)})t/\hbar<\beta'|T\exp$$
$$\{-(i/\hbar)\int_0^t ds\widetilde{H}_1(p,\beta,\beta';s)\}|\beta'>\exp\{(itH_n^{(0)})/\hbar\}|00Q>, \tag{2}$$

where $\widetilde{H}_1(p,\beta,\beta';s)$ is the hamiltonian in the interaction representation. It is constructed on basis of the unperturbed hamiltonian $H_0(p,\beta,\beta')$.

Further the factor under the integral sign of (2)

$$<\beta'|T\exp\left\{-(i/\hbar)\int_0^t ds\ H_1(p,\beta,\beta';s)\right\}|\beta'>,$$

is modified as follows;

$$1-(i/\hbar)\int_0^t ds\ Q'(s)\ G(s). \tag{3}$$

Here the operator $G(t)$ is defined in the following;

$$\frac{d}{dt}G(t)-i\Omega_{\beta p}^{(0)}G(t)=-(i/\hbar)Q'(t)-(1/\hbar^2)\int_0^t ds\{Q(t)\ Q(s)$$
$$+Q'(t)\ Q'(s)\}G(s) \tag{4}$$

with the initial condition $G(0)=0$, where $\Omega_{\beta p}^{(0)}=\Omega_\beta^{(0)}-\Omega_p^{(0)}$. $Q(t)$ and $Q'(t)$ is defined as follows;

$$Q(t)=v\ \exp\ (iH_n^{(p)}t/\hbar)\delta Q\ \exp(-iH_n^{(p)}t/\hbar)$$

and

$$Q'(t)=v\ \exp\ (iH_n^{(p)}t/\hbar)\delta Q'\ \exp(-iH_n^{(p)}t/\hbar).$$

It is assumed that the vibrational modes and the characteristic frequencies

change only slightly on the electronic excitations and that $\Delta_x=0$ except for $\Delta_{a_{1g}}$ for the lowest totally symmetric mode, where Δ_x measures the shift of the equiliblium configuration on the electronic excitation, belonging to the x-th symmetry species. Then with (3) the expression (2) are reduced to the following form;

$$I(\Omega)=\frac{1}{\pi}|<0|\boldsymbol{m}_e|\beta'>|^2\int_{-\infty}^{\infty}dt\ \exp\{it(\Omega-\Omega_\beta^{(0)})\}<00Q|\exp(-itH_n^{(p)}/\hbar)$$
$$\exp(itH_n^{(0)}/\hbar)|00Q>\Big\{1-(i/\hbar)v\int_0^t ds\ \exp(-i\omega s)$$
$$<00Q|\delta Q' G(s)|00Q>\Big\}. \tag{5}$$

The parts corresponding to the double phonon absorption and the double phonon emission, are dropped out of the factor $\{Q(t)Q(s)+Q'(t)Q'(s)\}$ of the expression (4). Then if $(iv/2\hbar)\Phi(z)$ represents the laplace transform of $<00Q|\delta Q' G(t)|00Q>$, $\Phi(z)$ is given by the following expression;

$$\Phi(z)=(z+i\omega)/\{(z^2+\omega^2)(z-i\Omega_{\beta\beta}^{(0)})+(3\alpha^2\omega^2/2)(z-i\omega)$$
$$+(\alpha^2\omega^2/2)(z+i\omega)\}, \tag{6}$$

where $\alpha^2=(v/\hbar\omega)^2$. The three zero points of the denominator in the above expression, are pure imaginary and are represented by $i\Omega_1$, $i\Omega_2$ and $i\Omega_3$, where $\Omega_1>\Omega_2>\Omega_3$. The inverse transform of (6) are substituted in the expression (5). Thus the following expression is obtained ;

$$I(\Omega)/\frac{1}{\pi}|<0|\boldsymbol{m}_e|\beta'>|^2=(V_{p\beta}^2/2)\zeta_p\Im\Big(\Omega-(\Omega_\beta^{(0)}+\omega-\Omega_1)\Big)$$
$$+\zeta_\beta\Im\Big(\Omega-(\Omega_\beta^{(0)}+\omega-\Omega_2)\Big)+(V_{p\beta}^2/2)\zeta'_\beta\Im\Big(\Omega-(\Omega_\beta^{(0)}+\omega-\Omega_3)\Big), \tag{7}$$

where $V_{p\beta}=v/\hbar(\Omega_1-\omega)$. $\Im(\Omega-\Omega')$ is defined as follows;

$$\Im(\Omega-\Omega')=\int_{-\infty}^{\infty}dt\ \exp\{it(\Omega-\Omega')\}<00Q|\exp(-itH_n^{(p)}/\hbar)$$
$$\exp(itH_n^{(0)}/\hbar)|00Q>, \tag{8}$$

On the right hand of (7), the first term corresponds to the intensity distribution of the ${}^1A_{1g}\rightarrow{}^1B_{1u}$ band system. The second term and third term correspond to the intensity distribution of the ${}^1A_{1g}\rightarrow{}^1E_{1u}$ band system.

Now $\overline{\Omega}_{p0}$ represents the average angular frequency of the ${}^1A_{1g}\rightarrow{}^1B_{1u}$ band system and $\overline{\Omega}_{\beta 0}$ represents the average angular frequency of the ${}^1A_{1g}\rightarrow{}^1E_{1u}$ band system. Then the ratio of the oscillator strength f_u of the ${}^1A_{1g}\rightarrow{}^1B_{1u}$ band system to the oscillator strength f_β of the ${}^1A_{1g}\rightarrow{}^1E_{1u}$ band system, is expressed as follows;

$$f_u/f_\beta=(\overline{\Omega}_{p0}/\overline{\Omega}_{\beta 0})\,\rho$$

and

$$\rho=(V_{p\beta}^2\,\zeta_p/2)\;/\left\{\zeta_\beta+(V_{p\beta}^2\,\zeta'_\beta/2)\right\}$$

The approximation which is adopted above, corresponds to the second approximation in the Lennard-Jones's form of perturbation theory.

§ 3. Results and Discussions

It is easily seen that the expression (5) shows the band progression[5]. The progression starts from Ω and extends to the shorter wave length side. Thus the ${}^1A_{1g}\rightarrow{}^1B_{1u}$ band system consists of the band progression which starts from $(\Omega_\beta^{(0)}+\omega-\Omega_1)$.

The ${}^1A_{1g}\rightarrow{}^1E_{1u}$ band system consists of the two band progressions, one of which starts from $(\Omega_\beta^{(0)}+\omega-\Omega_2)$. The other starts from $(\Omega_\beta^{(0)}+\omega-\Omega_3)$. It is noticed that the intensity of the latter band progression are much weaker than one of the former band progression because the factor $(V_{p\beta}^2/2)$ is included in the third term of the expression (7). It is observed that the ${}^1A_{1g}\rightarrow{}^1E_{1u}$ band system includes some members of the Rydberg sequence in the shorter wave length side[7]. If the contributions from the Rydberg sequence are excluded, f_β is estimated at 0.7 with the absorption spectra and thus f_u/f_β is estimated at 0.15 empirically[7]. Finally it is reasonable to choose 1.65 as the empirically estimated value of ρ. The theoretical curves of ρ versus $\Omega_{\beta p}^{(0)}/3\,\omega$ are shown in Fig.2.

The spacing between the first band of the ${}^1A_{1g}\rightarrow{}^1B_{1u}$ band system and that of the ${}^1A_{1g}\rightarrow{}^1E_{1u}$ band system, $\Delta\Omega$ is $\Omega_1-\Omega_2$. The spacing is estimated at 6000 cm^{-1} to 7000 cm^{-1} empirically[7][8]. In Fig. 3 the theoretical curves of $\Delta\Omega$ versus $\Omega_{\beta p}^{(0)}/3\,\omega$ are shown.

From Fig. 2 and 3, it is easily seen that the empirically estimated values of ρ and $\Delta\Omega$ are reproduced for $\alpha=2.5$ to 3 and for $\Omega_{\beta 0}^{(0)}/3\,\omega=0.75$ to 1.0. On the other hand M. H. Perrin et al estimate α at 1.5 semi-empirically and adopt $\Omega_{\beta p}^{(0)}/3\,\omega=1.0$. Finally they estimate f_u/f_β at 0.25. It is noted that they use the usual perturbation theory and that they proceed their calculation to the second order approximation. The value of α which is estimated by the present authors, is considerably larger than the semi-empirically estimated value of M. H. Perrin et al[3]. The value of $\Omega_{\beta p}^{(0)}$ which is estimated by the present authors, is almost equal to the value of M. H. Perrin et al[3][9]. It is important to note their following suggestion; in the semi-empirical calculations of electronic states such as the Pariser and Parr method which is applied to polyacenes, some fundamental parameters are estimated with the observed data of the ${}^1A_{1g}\rightarrow({}^1B_{1u}$ and ${}^1E_{1u})$ band

systems of benzene[10]. Then the observed spectroscopic data themselves should not be used but the parameters $\Omega_p^{(0)}$ and $\Omega_\beta^{(0)}$ which are estimated from the ob-observed spectroscopic data, should be used. This kind of calculation of electronic states, is based on the Born-Oppenheimer approximation. When this approximation is violated, the observed spectra can not be interpreted on basis of the Born-Oppenheimer approximation[11]. Thus the above comments are accepted. In this article the present authors' calculation shows that $a\omega \approx \Omega_{\beta p}^{(0)}$. Hence it is necessary to proceed the calculation to a higher approximation.

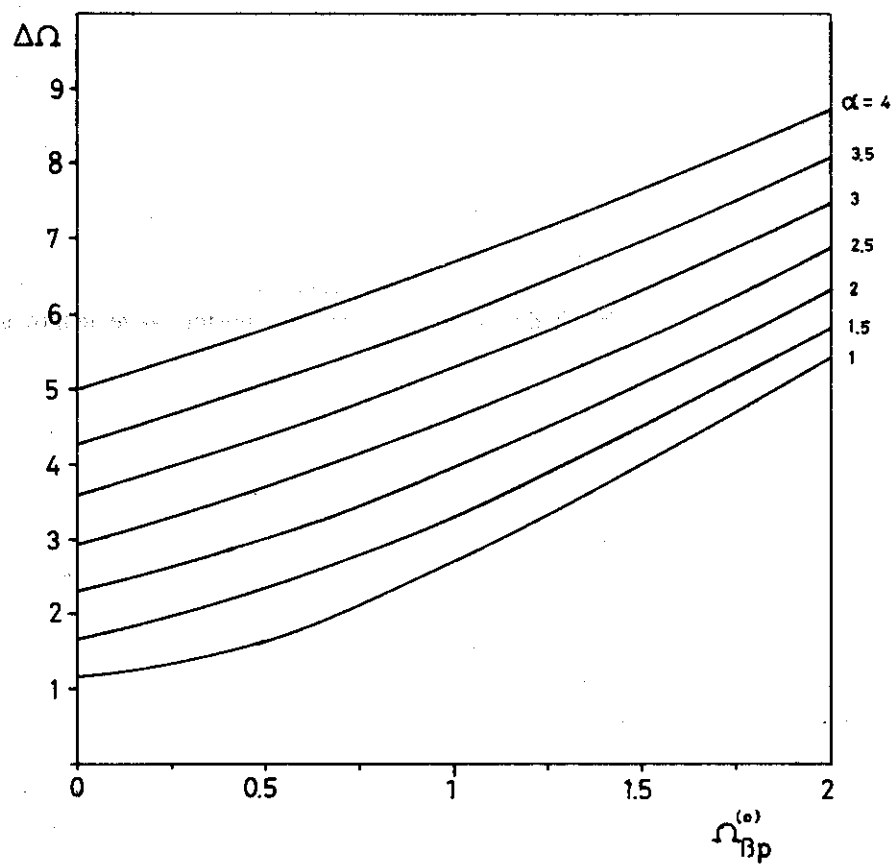


Fig. 2. The spacing between the first peak of the $^1A_{1g} \rightarrow {}^1B_{1u}$ band system and one of the $^1A_{1g} \rightarrow {}^1E_{1u}$ band system. The abscissa scale and the ordinate scale are $\Omega_{\beta p}^{(0)}/3\omega$ and $\Delta\Omega/\omega$ respectively.

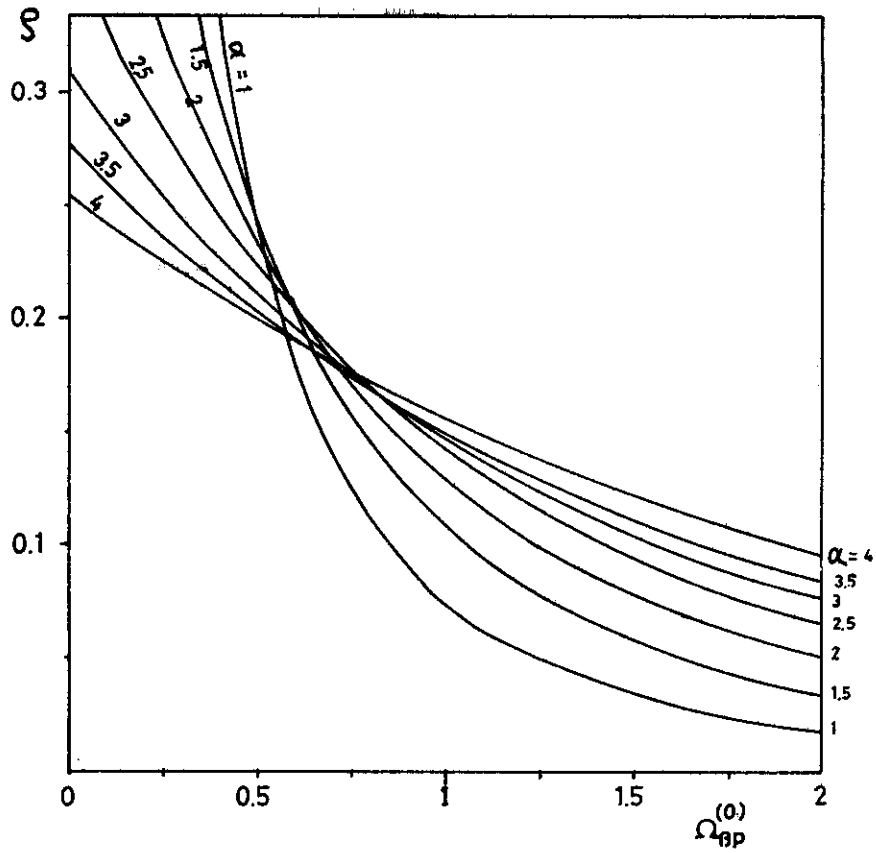
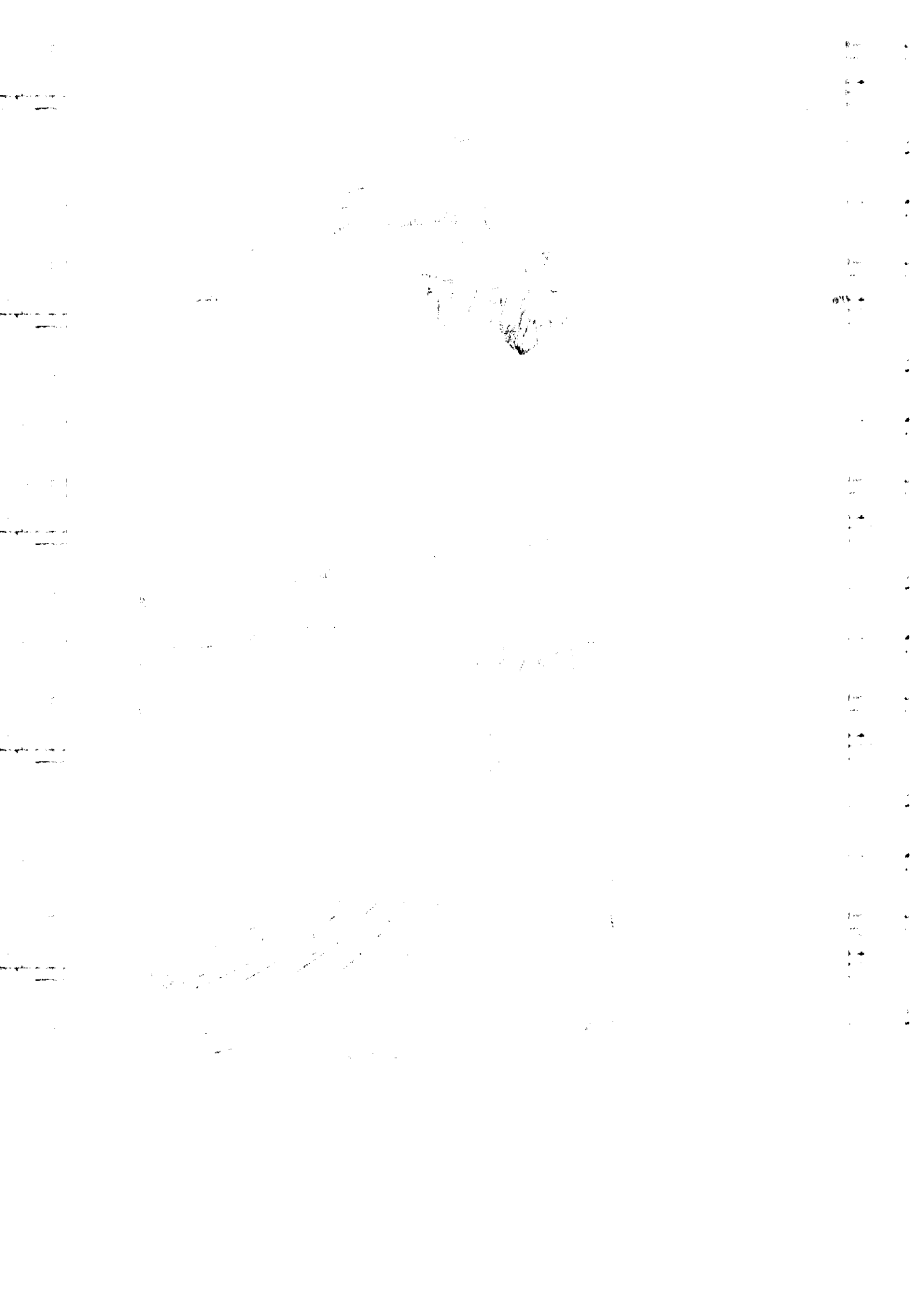


Fig. 3. The parameter of intensity ratio ρ.
The abscissa scale is $\Omega^{(0)}_{\beta\beta}/3\omega$.

References

1) A. D. Liehr, Z. Naturforschg. **16a** (1961), 641.
2) H. C. Longuet-Higgins, Advan. Spectry. **2** (1961), 429.
3) M. H. Perrin, M. Gouterman and C. L. Perrin, J. Chem. Phys. **50** (1969), 4137.
4) J. H. van der Waals, A. M. D. Berghuis and M. S. de Groot, Molec. Phys. **13** (1967), 301. J. H. van der Waals, A. M. D. Berghuis and M. S. de Groot, Molec. Phys. **21** (1971), 497.
5) Yu. E. Perlin, Sov. Phys. Usp. **6** (1964), 542.
6) T. Ōtsu and T. Watanabe, Phys. Rep. Kumamoto Univ. **1** (1973), 35.
7) V. V. Bertsev, G. Yo. Zelikina and T. G. Meister, Opt. Spectrosc. **36** (1974), 168.
8) T. N. Bolotnikova and O. F. Elnikova, Opt. Spectrosc. **36** (1974), 168.
9) W. J. Pott, J. Chem. Phys. **23** (1955), 73.
10) R. Pariser, J. Chem. Phys. **24** (1956), 250.
11) W. E. Donath, J. Chem. Phys., **42** (1965), 118.



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A Simple and Versatile Digital Pulse Generator for Pulsed NMR Experiment

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For a pulse NMR experiment, many kinds of pulse sequence are used.[1] We have constructed a very simple and versatile trigger pulse generator, using a digital circuit.[2] Intervals, numbers and any configuration of pulses for various NMR experiment can be easily obtained by this apparatus.

This is composed of the following four main units, (a) clock time generator unit, (b) base time unit, (c) preset counter units and (d) monostable multi-vibrator units. A crystal oscillator (1MHz) which has an relative accuracy of about 10^{-7} is used in the clock time generator. Using decimal counters, clock pulse with the periode of 10^{-6} to 10^{2} sec is available for (b) and (c) units. The (b) unit is used to determine the repetition time of a series of pulses. The (c) unit is composed of 3 syncronized reversible (up/down) counters (Texas Instruments Co. SN74190) which are operated in a down count mode. In order to preset a counting number of the counter, thum-wheel switches are also used. This unit has a clock pulse terminal, start terminals, stop terminals, output terminals and BCD input terminals as seen in Fig. 1(A). When the first trigger pulse is applied to the start terminal, a counting operation begins and when the second trigger pulse is applied to the stop terminal, the operation stops and the unit returns to the initial state. When the counting number of the counter becomes zero and return to the preset number, a short pulse appers at the output terminals. If the output terminal and the stop terminal are linked together by wire in one preset counter unit, two basic operations, (A) $\tau_1+\tau_2$ and (B) $\tau\times n$ are obtained as shown in Fig.1. Here τ is the time of the preset number multiplied by the periode of the clock pulses. By an appropriate combination of (A) and (B) operation, many kinds of trigger pulse sequence are obtained, for example, $\tau_1\times n+\tau_2$, $(\tau_1+\tau_2)\times n$, etc. It should be noticed that $(\tau_1+\tau_2)\times n\neq\tau_1\times n+\tau_2\times n$. We now study the Carr-Purcell technique. For this experiment, a trigger pulse sequence of $\tau+2\tau\times n$ is needed and is obtained easily by use of this system as seen in Fig.2. This trigger pulse generator is introduced to the monostable multi-vibrator where the first pulse is 90° pulse and

the others are 180° pulses. Figure 3 shows the typical view of recorder trace of the echo signals in the resonance of proton of H_2O.

Since the way of the linking between the terminals are basically ×, +, (and), the system can be easily developed so as to connect automatically by writing a formulae on a key pannel.

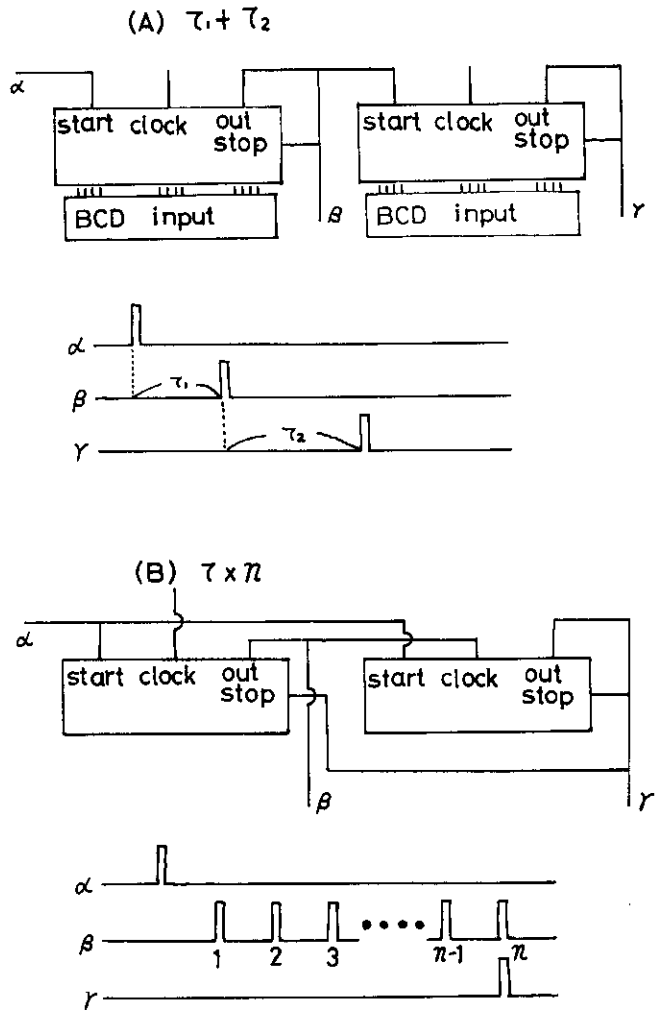

Fig. 1 Methods of linking between preset counter units in order to make basic operations (A) and (B), and their time charts.

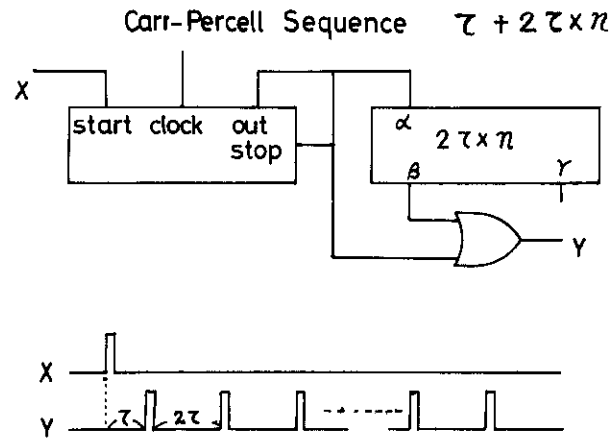

Fig. 2 A method of making a pulse sequence for Carr-Purcell experiment and it's time chart.

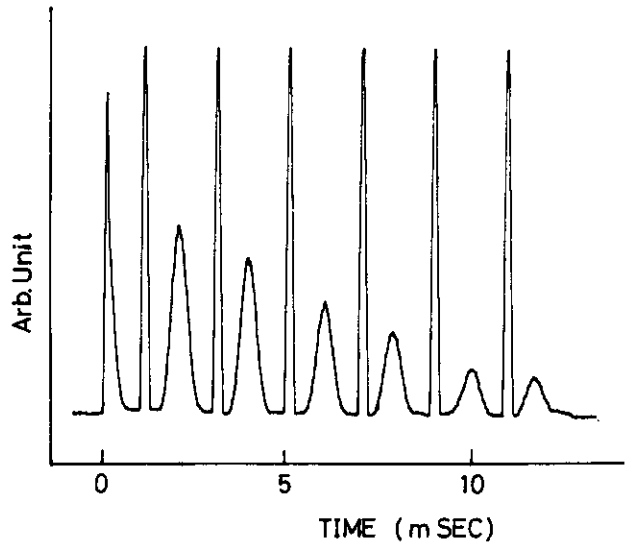

Fig. 3 A recorder trace of echo signals in the Carr-Purcell experiment where the interval of pulses is 1.5 m sec. Here Y-axis denotes an intensity of the echo signals in arbitary unit and X-axis denotes time.

References

1) "Advances in Magnetic Resonance" ed. J. S. Waugh (Academic Press, New York and London) *Vol. 1-8.*
2) Texas Instruments Asia Limited, "TTL Application Mannual ©" (Electron Digest, 1974)
3) H. Y. Carr and E. M. Purcell, Phys. Rev. **94** (1954) 630.

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