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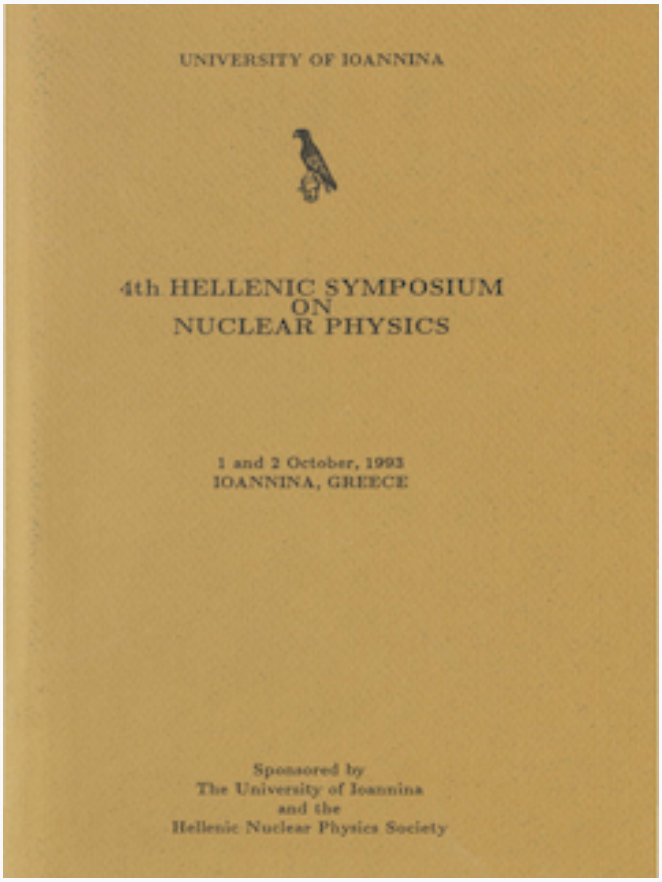

Approximate treatment of the Dirac equation with scalar and vector potentials of rectangular shapes

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Approximate treatment of the Dirac equation with scalar and vector potentials of rectangular shapes

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Abstract

The Dirac equation with scalar potential $U_S(r)$ and fourth component of vector potential $U_V(r)$ is considered in the case of the rectangular shapes of these potentials with the same radius R and approximate analytic expressions are derived for the single-particle energy of bound states in certain cases. The results obtained with these expressions are compared with the corresponding "exact" results obtained by solving the eigenvalue equation numerically.It is found that very good results are obtained for the ground state and for quite a wide range of values of R with one of the proposed expressions. Even the corresponding non-relativistic version of this expession, has not been derived before, to our knowledge.

The Dirac equation with scalar potential $U_S(r)$ and fourth component of vector potential $U_V(r)$ [1,2]

$$[c\vec{\alpha}\vec{p} + \beta\mu c^2 + \beta U_S(r) + U_V(r)]\Psi = E\Psi \tag{1}$$

has attracted much interest in the past years (see refs. 2,3 and references therein). In this equation $\vec{\alpha}$ and β are the usual Dirac matrices, Ψ the Dirac spinor and E the total energy $E = \varepsilon + \mu c^2$.

By expressing the Dirac spinors in terms of the large (G) and small (F) component:

$$\Psi = \Psi_{Nljm} = \begin{pmatrix} \frac{iG_{Nlj}(r)}{r} \\ \frac{F_{Nlj}(r)\vec{\sigma}\vec{r}}{r} \end{pmatrix} \varphi_{ljm} \tag{2}$$

+Presented by C. G. Koutroulos.

where

$$\varphi_{ljm} = (Y_l^{m_l} \otimes \chi_{1/2}^{m_s})_{jm} \tag{3}$$

and $\chi_{1/2}^{m_s}$ are the Pauli spinors, one may derive from (1) the following Schrodinger-type equation (for central potentials) [4]

$$g''(r) - \left[\frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}(V_{centr} + V_{s.o.} - \varepsilon)\right] g(r) = 0 \tag{4}$$

where

$$g(r) = D^{-1/2}(r)G(r)$$

$$D(r) = \frac{1}{\hbar c}(2\mu c^2 + \varepsilon + U_-(r)) \tag{5}$$

G is the large component of the Dirac wave function and

$$V_{centr} = U_+(r) + \frac{\hbar^2}{2\mu}[\frac{1}{\hbar^2 c^2}[U_+(r) - \varepsilon][U_-(r) + \varepsilon] -$$
$$D^{-1}(r)D'(r)r^{-1} - [2D(r)]^{-1}D''(r) + \frac{3}{4}D^{-2}(r)[D'(r)]^2] \tag{6}$$

$$V_{s.o}(r,\varepsilon) = -\frac{\hbar}{2\mu}\frac{1}{[2\mu c^2 + \varepsilon + U_-(r)]}\frac{1}{r}\frac{dU_-(r)}{dr}\vec{l}\vec{\sigma} \tag{7}$$

The potentials $U_\pm(r)$ are defined as follows

$$U_\pm(r) = U_S(r) \pm U_V(r) \tag{8}$$

We consider the case in which $U_+(r)$ and $U_-(r)$ are square wells with the same radius R [5] and depths D_+ and D_- respectivelly i.e.

$$U_\pm(r) = -D_\pm[1 - \Theta(r - R)] \tag{9}$$

where Θ is the unit step function.

Square-well potentials, in particular of infinite depth, have been used in applications of non-relativistic Quantum Mechanics in spite of their crudeness because of the analytic expressions to which they lead. As it was also pointed out recently [6] the eigenvalues of the one-dimensional Schrodinger equation with a potential which is a sum of even powers of x may be calculated, by using the eigenfunctions and eigenvalues of the infinite square well.

The generalized Dirac equation with the square well potentials we are discussing may be solved analytically, for every bound state [7]. The expressions for G and F are given in terms of spherical Bessel functions j_l and spherical Hankel functions of the first kind $h_l^{(1)}$ and are the following

$$G(r) = \tilde{N} nr \left[[1 - \Theta(r-R)] j_\ell(nr) + \Theta(r-R) \frac{j_\ell(nR)}{h_\ell^{(1)}(in_0R)} h_\ell^{(1)}(in_0 r) \right] \tag{10}$$

$$\begin{aligned} F(r) = & \\ & \tilde{N} nc\hbar \Big[[1 - \Theta(r-R)] \frac{1}{\varepsilon + 2\mu c^2 - D_-} [nr j_{\ell-1}(nr) + (k-\ell) j_\ell(nr)] + \\ & \Theta(r-R) \frac{1}{\varepsilon + 2\mu c^2} \frac{j_\ell(nR)}{h_\ell^{(1)}(in_0R)} \left[in_0 r h_{\ell-1}^{(1)}(in_0 r) + (k-\ell) h_\ell^{(1)}(in_0 r) \right] \Big] \end{aligned} \tag{11}$$

while the energy eigenvalue equation is [7]

$$\left[1 - \frac{D_-}{2\mu c^2 + \varepsilon} \right] \frac{in_0 R h_{l-1}^{(1)}(in_0 R)}{h_l^{(1)}(in_0 R)} = \frac{(k-l) D_-}{2\mu c^2 + \varepsilon} + \frac{nR j_{l-1}(nR)}{j_l(nR)} \tag{12}$$

In these expressions the quantities n and n_0 are defined as follows:

$$n = \left[\frac{2\mu}{\hbar^2} (D_+ + \varepsilon)(1 - (D_- - \varepsilon)(2\mu c^2)^{-1}) \right]^{1/2} \tag{13}$$

$$n_0 = \left[\frac{2\mu}{\hbar^2} [-\varepsilon(1 + \varepsilon(2\mu c^2)^{-1})] \right]^{1/2} \tag{14}$$

and $k = \pm(j + 1/2)$ for $j = (l \mp 1/2)$. The quatum numbers in G, F, ε and $\tilde{N}$ have been suppressed.

The disantvandage with eigenvalue equation (12) is that in general can not be solved for ε and thus it is not possible to have an explicit expression of the energy in terms of the potential parameters. We show in this letter, however, that in certain cases this can be achieved approximately in a rather satisfactory way. Thus, one is led to fairly simple approximate analytic expressions for ε. Before proceeding we recall that usually in practice D_- is quite smaller than $2\mu c^2$ and D_+ much smaller than D_-.

Let us consider the case in which nR and n_0R are sufficiently larger than $\frac{l}{2}(l+1)$ [see also refs. 8,9] so that we may use the following asymptotic form for $j_l(nR)$ and $h_l^{(1)}(in_0R)$

$$j_l(nR) \simeq \frac{1}{nR} sin(nR - \frac{l\pi}{2}) \ , \qquad h_l^{(1)}(in_0R) \simeq \frac{-1}{n_0R} e^{-n_0R - il\frac{\pi}{2}} \tag{15}$$

Thus, eq. (12) may be written in the form:

$$n_0R + nRcot(nR - \frac{l\pi}{2}) = \frac{D_-}{2\mu c^2 + \varepsilon}[n_0R - (k-l)] \tag{16}$$

It is seen immediately that for the ground state : $1s_{\frac{1}{2}}$, $(l = 0, k = -1)$ this equation coincides with the exact eigenvalue equation for this state (see appendix of ref. [5]).For the excited states, however, it is approximate.

Eq. (16) may be written in the following form which is suitable for our treatment:

$$n^2R^2 = \frac{2\mu}{\hbar^2}D_+R^2(1 + C_R)sin^2[(2N + l)\frac{\pi}{2} - nR] \tag{17}$$

where $N = 1, 2, 3, ...,\ \ l = 0, 1, 2, ...$ and

$$C_R = [\frac{\varepsilon}{D_-} - \frac{\varepsilon}{D_+} - 1]D_-(2\mu c^2)^{-1} + \frac{1}{\frac{2\mu}{\hbar^2}D_+R^2}\left[-(n_0R)^2 + [n_0R(1 - \frac{D_-}{2\mu c^2 + \varepsilon}) + \frac{(k-l)D_-}{2\mu c^2 + \varepsilon}]^2\right] \tag{18}$$

We are interested in the case of a well of sufficiently large depth D_+ and radius R.Thus if we write eq. (17) in terms of the *arcsin* of the small quantity

$$x = nR[(2\mu/\hbar^2)D_+R^2(1 + C_R)]^{-1/2}$$

we may keep only the leading term in the expansion of $arcsinx$ and obtain the eigenvalue equation in the approximate form

$$(nR)^2 = \frac{(2N + l)^2\pi^2}{4(1 + \lambda_R)^2} \tag{19}$$

where

$$\lambda_R = \lambda_0[1 + C_R]^{-1/2}\ \ (a), \qquad \lambda_0 = (\frac{2\mu}{\hbar^2}D_+R^2)^{-1/2}\ \ (b) \tag{20}$$

It is interesting to note that if we neglect completely the terms of order $(2\mu c^2)^{-1}$ the eigenvalue equation (12) goes over to the corresponding non relativistic one.In this case equ. (19) may be written in the form

$$\varepsilon_{NR_l} = -D_+ + \frac{\hbar^2}{8\mu}\frac{(2N + l)^2\pi^2}{(1 + \lambda_0)^2R^2} \tag{21}$$

This is an approximate expression of the non-relativistic energy for a particle of mass μ in a square-well potential of depth D_+ and radius R.In the case of the s-states the above

expression reduces to a known approximate expression [10] derived from the corresponding Schrodinger eigenvalue equation.

An approximate relativistic expression for the energy may be derived from expression (19) if the unknown energy which appears in terms which are expected to be small is estimated by means of (21).In this way we obtain the following approximate expression for the relativistic energy which we shall denote by ε_{R1}

$$\varepsilon_{R_1} = -D_+ + \frac{\hbar^2}{8\mu^*_{g_1}} \frac{(2N+l)^2\pi^2}{(1+\lambda_{R1})^2 R^2} \tag{22}$$

where $\mu^*_{g_1}$ is a sort of "effective mass" given by

$$\mu^*_{g_1} = \mu[1 + (\varepsilon_{NR1} - D_-)(2\mu c^2)^{-1}] \tag{23}$$

and λ_{R1} is given by (20a) in which the energy in the expression of C_R has been substituted by ε_{NR1} (expression (21)). The above procedure may be iterated. Thus we may use as expressions for the energy in $\mu^*_{g_1}$ and λ_{R_1} which appear in (22) and (23) the ones obtained in the previously described way and so on.

An improved expression for ε may be obtained if instead of retaining only the leading term x in the expansion of $arcsinx$:

$$\begin{aligned} arcsinx &= x + \frac{x^3}{2\cdot 3} + \frac{1\cdot 3}{2\cdot 4\cdot 5}x^5 + ... \\ &= x(1+F(x)) \end{aligned} \tag{24}$$

that is , instead of setting $F(x) = 0$ we write, as in a similar expansion, $F(x) \approx F(x^{ap})$ where x^{ap} is the expression resulting from the eigenvalue equation solved approximately with $arcsinx \approx x$.This procedure leads in the nonrelativistic case to the following expression for the energy which we shall denote by ε_{NR_2} i.e.

$$\varepsilon_{NR_2} = -D_+ + \frac{\hbar^2}{8\mu} \frac{(2N+l)^2\pi^2}{(1+F_0)^2 R^2} \tag{25}$$

where

$$F_0 = \frac{arcsin(\lambda_0(2N+l)\pi/(2(1+\lambda_0)))}{(2N+l)\pi/(2(1+\lambda_0))} \tag{26}$$

In the relativistic case the corresponding expression is

$$\varepsilon_{R_2} = -D_+ + \frac{\hbar^2}{8\mu^*_{g_2}} \frac{(2N+l)^2\pi^2}{(1+F_{R_2})^2 R^2} \tag{27}$$

where

$$F_{R_2} = \frac{arcsin(\lambda_{R_2}(2N+l)\pi/(2(1+\lambda_{R_2})))}{(2N+l)\pi/(2(1+\lambda_{R_2}))} \tag{28}$$

$$\mu^*_{g_2} = \mu[1+(\varepsilon_{NR2} - D_-)(2\mu c^2)^{-1}] \tag{29}$$

and λ_{R_2} is given by (20α) in which the energy in the expression of C_R has now been estimated with ε_{NR_2} (expression (25)).

We discuss also the case of states for which in addition $|\varepsilon| \ll D_+$.This condition is satisfied for loosely bound states in a sufficiently deep well.In this case it may be seen from equ. (16), in analogy with the corresponding non-relativistic treatment [10], that the cotangent should be close to zero.Thus, we arrive at the following approximate expression

$$\varepsilon_{R_3} = 2D_+[-1+\tilde{\lambda}_0(2N+l-1)\frac{\pi}{2}] \tag{30}$$

where

$$\tilde{\lambda}_0 = \lambda_0(\frac{\mu}{\mu^*_{g_3}})^{1/2} \tag{31}$$

and $\mu^*_{g_3}$ is calculated from the expression of

$$\mu^*_g = \mu[1+(\varepsilon - D_-)(2\mu c^2)^{-1}] \tag{32}$$

by using for the energy the corresponding non-relativistic expression [10]

$$\varepsilon_{NR_3} = 2D_+[-1+\lambda_0(2N+l-1)\frac{\pi}{2}] \tag{33}$$

Expressions (30) and (33) gave usually poor results in the cases we studied.However an alternative expression which gives considerably improved results in a variety of cases (see below) may be derived by using expression (17) and the following expansion for the $arcsin(1-z)$ (see expression 4.4.42 of ref.[11]):

$$arcsin(1-z) = \frac{\pi}{2} - (2z)^{1/2}[1+\sum_{k=1}^{\infty}\frac{1\cdot 3\cdot 5\cdots(2k-1)}{2^{2k}(2k+1)k!}z^k] \tag{34}$$

$$|z| < 2$$

We write on the basis of eqs.(17) and (33):

$$(2N+l)\frac{\pi}{2} - nR = arcsin(\lambda_R nR) \simeq \frac{\pi}{2} - (2z)^{\frac{1}{2}}(1+\frac{z}{12}) \tag{35}$$

where $\lambda_R nR = 1 - z$. This equation may be easily solved to a good approximation with respect to $1 - z$ for z sufficiently small. Such a procedure has not been followed, to our knowledge, even in the non relativistic case. The final result for the energy eigenvalue is

$$\varepsilon_{R_4} = -D_+ + \frac{\hbar^2}{2\mu_g^*}\frac{\theta_{Nl}^2}{R^2} \tag{36}$$

where

$$\theta_{Nl} = [\frac{(4\lambda_R - 3\alpha_{Nl})}{(\lambda_R^2 - 3)}[1 + (1 - \frac{(\lambda_R^2 - 3)(7 - 3\alpha_{Nl}^2)}{(4\lambda_R - 3\alpha_{Nl})^2})^{\frac{1}{2}}]] \tag{37}$$

with $\alpha_{Nl} = (2N + l - 1)\frac{\pi}{2}$.

The energies entering in μ_g^* and λ_R may be evaluated by using for ε the ε_{NR_4} which is of the same structure as (36) but with μ instead of μ_g^* and with λ_0 instead of λ_R in the expression of θ_{Nl}.

In order to test the accuracy of the approximate expressions ε_{R_1} and ε_{R_2}, numerical calculations have been performed and the results were compared with those obtained by solving numerically the eigenvalue equation (12). The following values of the parameters were used (see ref.[5]) $D_+ = 30.55MeV$, $D_- = 300MeV$ and $R = r_0 A_{core}^{1/3}$ ($r_0 = 1.01fm$) A_{core} being the mass number of the core nucleus. These are rather reasonable values for the potential parameters of a Λ particle in its ground state in hypernuclei.It should be noted that there is no much difference if the values $D_+ = 30.77MeV$, $D_- = 443MeV$ *and* $r_0 = 1.022fm$ are used instead.

The results obtained for the $1s_{1/2}$,$1p_{3/2}$ and $1d_{5/2}$ states and for various values of R (and therefore of λ_0) are displayed in table 1. The results for the states $1p_{1/2}$ and $1d_{3/2}$ are usually rather similar. The smallest value of A_{core} used corresponds to ${}^{12}_{\Lambda}C$ while the largest to ${}^{208}_{\Lambda}Pb$. In each case the values of the "exact" relativistic energy ε_{ex} for the rectangular potentials that is the one obtained by solving numerically the eigenvalue equation (12) and the approximate ones ε_{R_1} and ε_{R_2} are shown. In addition the quantities nR and n_0R calculated with ε_{ex} are also displayed. It is seen from the results of this table that for the $1s$ and $1p$ states and mainly for the larger values of R which correspond also to larger values of nR and n_0R the approximate expressions ε_{R_1} and ε_{R_2} are good approximations to ε_{ex}. From the same table it is also seen that the results with ε_{R_2} are better compared to those obtained with ε_{R_1}. In some cases the improvement is considerable.

In table 2 the results obtained with ε_{R_4} are displayed for various states and values of R and are compared with those obtained with the numerical solution of the eigenvalue equation. It is seen that for the ground state the accuracy of ε_{R_4} is very good both for the

smaller and for the larger values of R. We further observe from both tables that for the higher states the accuracy of the various approximate expressions is deteriorating quite rapidly.It should be noted, however, that the accuracy dependes on the values of D_+ and R.If in a physical problem the values of these quantities were larger, the accuracy for each state should have been improved.

We may conclude that the analytic expressions ε_{R_1} and ε_{R_2} give, in a number of cases, single particle enegry values which are fairly close to those obtained from the numerical solution of the eigenvalue equation ,derived by means of the Dirac equation with potentials U_S and U_V of rectangular shape and of the same radius. Expression ε_{R_4} gives in some of these cases better results than those obtained with the above mentioned expressions and in particular with ε_{R_1}.

References

1. H.P.Duerr Phys. Rev 103 (1956) 469.

2. Rajat K. Bhaduri Models of the Nucleon (From Quarks to Soliton), Lecture notes and supplements in Physics, chapter 2, Adison-Wesley, N. Y. (1988).

3. B. D. Serot and J. D. Walecka in Advances in Nuclear Physics ed. by J. W. Negele and E.Vogt (Plenum, New York, 1986 Vol 16;)

4. R. Brockmann, Phys. Rev. C18, (1978) 1510 and references therein.

5. C. G. Koutroulos and M. E. Grypeos Phys. Rev. C 40, (1989) 275

6. M.A.M. de Aguiar and A.L. Xavier J.. Physics Letters A 164 (1992) 279.

7. G.J. Papadopoulos, C.G. Koutroulos, M. E. Grypeos "Proc. of the Second Hellenic Symposium on Nuclear Physics" p.389, Athens 1991 and submitted for publication.

8. L. Schiff "Quantum Mechanics", 3rd edition,p.86 McGraw Hill (1984).

G.N. Watson "Theory of Bessel functions " 2nd ed. p. 199 Mc Millan (N.Y) (1945).

9. Stephen Gasiorowicz QuantumPhysics p. 187, John Wiley and Sons, N.Y. (1974).

10. C.D.Cantrell Am. Journal of Physics 39, (1971) 107.

11. M. Abramowitz and I. A. Segun Handbook of Mathematical functions, p.82, Dover publications (1968).

Table 1

Energy eigenvalues of various states obtained with D_+=30,55 MeV D_-=300 MeV and various values of R ($R=1.01\ A^{1/3}$ fm). The values obtained with the numerical solution of the eigenvalue equation (12) are denoted by ε_{ex} while those obtained with the approximate expressions by ε_{R1} and ε_{R2} (see text for these expressions and also for the expressions of $\underline{\lambda}_o$, nR and n_oR).

	$1s_{1/2}$							$1p_{3/2}$					$1d_{5/2}$				
A_{core}	R	$\underline{\lambda}_o$	nR	n_oR	$-\underline{\varepsilon}_{ex}$	$-\underline{\varepsilon}_{R1}$	$-\underline{\varepsilon}_{R2}$	nR	n_oR	$-\varepsilon_{ex}$	$-\varepsilon_{R1}$	$-\varepsilon_{R2}$	nR	n_oR	$-\varepsilon_{ex}$	$-\varepsilon_{R1}$	$-\varepsilon_{R2}$
12	2.31	0.35	2.14	1.76	11.2	9.2	11.8										
15	2.49	0.31	2.21	2.07	13.1	11.6	13.4										
39	3.45	0.22	2.47	3.61	19.8	19.4	19.8	3.4	2.5	9.5	5.5	9.0					
50	3.72	0.21	2.50	4.03	21.1	20.8	21.1	3.5	3.0	11.9	8.8	10.9	4.1	1.1	1.6		
88	4.49	0.17	2.60	5.16	23.6	23.5	23.6	3.7	4.3	16.7	14.8	15.6	4.7	3.1	8.4		
137	5.21	0.15	2.68	6.18	25.1	25.1	25.1	3.8	5.5	19.7	18.3	18.7	4.8	4.5	13.0	8.8	10.5
207	5.98	0.13	2.72	7.27	26.3	26.2	26.3	3.9	6.6	21.9	21.0	21.1	4.9	5.8	16.5	13.5	14.3

Table 2

Energy eigenvalues of various states obtained with $D_+ = 30.55 MeV$, $D_- = 300 MeV$ and various values of R ($R = 1.01 A_{core}^{1/3} fm$).The values obtained with the numerical solution of the eigenvalue equation (12) are denoted by ε_{ex} while those obtained with the approximate expression by ε_{R_4} (see text).

A_{core}	$s_{1/2}$ $-\varepsilon_{R_4}$	$s_{1/2}$ $-\varepsilon_{ex}$	$p_{3/2}$ $-\varepsilon_{R_4}$	$p_{3/2}$ $-\varepsilon_{ex}$	$p_{1/2}$ $-\varepsilon_{R_4}$	$p_{1/2}$ $-\varepsilon_{ex}$	$d_{5/2}$ $-\varepsilon_{R_4}$	$d_{5/2}$ $-\varepsilon_{ex}$	$d_{3/2}$ $-\varepsilon_{R_4}$	$d_{3/2}$ $-\varepsilon_{ex}$
12	11.3	11.2								
15	13.2	13.1								
19	15.1	15.0	1.4	1.8	0.3	0.5				
27	17.6	17.5	4.4	5.6	3.2	4.5				
31	18.5	18.4	5.8	7.12	4.7	6.1				
39	19.8	19.8	8.1	9.5	7.3	8.7				
50	21.1	21.1	10.6	11.9	9.9	11.3				
88	23.6	23.6	15.5	16.7	15.2	16.3	5.5	8.4	4.5	7.5
137	25.2	25.1	18.7	19.7	18.5	19.4	10.3	13.0	9.6	12.4
207	26.3	26.3	21.1	21.9	21.0	21.8	14.2	16.5	13.8	16.2