

## **k-State Solutions for the Fermionic Massive Spin-1/2 Particles: Thermodynamic Properties and Information Entropy Under the Shifted Tietz-Wei Potential**

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### *Abstract*

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*We have approximately solved the Dirac equation for the Shifted Tietz-Wei potential including a Coulomb-like tensor interaction with arbitrary spin-orbit coupling quantum number  $k$ . In the frame work of spin and pseudospin symmetry, we obtained the energy eigenvalue equations and their corresponding eigenfunctions in a closed form by using the supersymmetric approach. We have equally computed the Shannon entropy, Renyi entropy, Onicesu energy and Fisher information entropy of the Shifted Tietz-Wei potential. The numerical results show that the Coulomb-like tensor interaction removes degeneracies between spin and pseudospin state doublets.*

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### **1.0 Introduction**

In the recent time, there has been a renewed interest in solving the Dirac equation analytically to describe the relativistic spin-1/2 particles [1]. It is well known that the analytical solutions of the Dirac equation for  $k = 0$  cannot be possible for some potential models such as the Coulomb potential [2, 3], Harmonic oscillator [4], Yukawa potential [5, 6], inversely quadratic Yukawa potential [7], Hellmann potential [8-11]. However, for  $k = 0$ , the analytical solutions can be obtained for a number of potentials. The Dirac equation as well, is the most perfect example of a relativistic wave equation which is able to describe in a simple manner, the relativistic effects due to the spin of particles [12]. In the strong coupling case, relativistic effects have been rarely discussed, primarily due to difficulties involved in solving analytically the Dirac equation. Several model potentials have been introduced recently to explore the relativistic energy spectra and wave function behaviour [13]. In the case that the scalar potential equal to vector potential, Hu and Su [14] obtained the exact solution or the s-wave Dirac equation for Hulthén potential. Hout et al. [15] and Chen [16] gave exact solutions of the Dirac equation with Morse and wood-saxon potentials respectively. The Dirac equation has been studied under spin and pseudospin symmetry to explain the features of deformed nuclei [17], superdeformation [18], magnetic moment interpretation [19, 20], identical bands [21, 22] and establish an effective shell-model coupling scheme [23]. To the subject of our knowledge, the symmetry limits and thermodynamic properties as well as the information entropy of the Shifted Tietz-Wei potential has not be studied yet. These, call for further research studies. In this paper, we examine the spin and pseudospin symmetry with the Shifted Tietz-Wei potential, the interaction of the potential with the thermodynamic properties and the information entropy. The Shifted Tietz-Wei potential have been studied by Falaye et al. [24] under the D-dimensional Schrödinger equation in the framework of exact quantization rule. The shifted Tietz-Wei potential is related to the Tietz-Wei potential and the Morse potential model. The shifted Tietz-Wei potential is closely related to the Morse potential function for large values of  $r$  in the regions  $r \approx r_e$  and  $r > r_e$  but different at  $r \approx 0$  [24]. This potential (shifted Tietz-Wei potential) is as good as the traditional Morse potential and better than the Tietz-Wei potential in stimulating the atomic interaction for diatomic molecules [26]. The shifted Tietz-Wei potential is given as [24].

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$$V_{STW}(r) = D_e \left[ \frac{2(C_h - 1)e^{-b_h(r-r_e)} - (C_h^2 - 1)e^{-2b_h(r-r_e)}}{(1 - C_h e^{-b_h(r-r_e)})^2} \right]^2, \quad (1)$$

where  $b_h = \beta(1 - C_h)$ ,  $r_e$  is the molecular bond length,  $\beta$  is the Morse constant,  $D_e$  is the potential well depth,  $C_h$  is the optimization parameter and  $r$  is the internuclear distance. This paper is organized as follows. In section 2, we briefly introduce the Dirac equation with scalar and vector potential with arbitrary spin-orbit coupling quantum number  $k$  including tensor interaction under spin and pseudospin symmetry limits. The energy eigenvalue equations and the corresponding eigenfunctions are obtained in section 3. In this section, we obtained the non-relativistic limit of the spin symmetry. In section 4, we calculate the thermodynamic properties. In section 5, we compute the information entropy, present numerical results and some remarks. Finally, our conclusion is given in section 6.

## 2.0 Dirac Equation

In this section, we briefly review the Dirac equation. The Dirac equation with scalar  $S(r)$  and  $V(r)$  potentials in spherical coordinates is given as [25-27]

$$\left[ \vec{\alpha} \cdot \vec{p} + \beta(M + S(r)) - (E - V(r)) \right] \psi(\vec{r}) = 0, \quad (2)$$

where  $\vec{p} = -i\vec{\nabla}$  is the momentum operator,  $E$  denote the relativistic energy of the system,  $\alpha$  and  $\beta$  are  $4 \times 4$  usual Dirac matrices. For a particle in a spherical field, the total angular momentum operator  $j$  and the spin-orbit matrix operator  $k = (\sigma \cdot L + 1)$ , where  $\sigma$  and  $L$  are the Pauli matrix and orbital angular momentum respectively, commute with the Dirac Hamiltonian. The eigenvalues of  $k$  are  $k = -(j + 1/2)$  for the aligned spin ( $s_{1/2}, p_{3/2}, etc$ ) and  $k = (j + 1/2)$  for the unaligned spin ( $p_{1/2}, d_{3/2}, etc$ ). The complete set of conservative quantities can be chosen as  $(H, K, J^2, J_z)$ . The Dirac spinor is [25, 26]

$$\psi_{nk}(r) = \begin{pmatrix} f_{nk}(r) \\ g_{nk}(r) \end{pmatrix} = \begin{pmatrix} \frac{F_{nk}(r)}{r} Y_{jm}^l(\theta, \vartheta) \\ \frac{G_{nk}(r)}{r} Y_{jm}^i(\theta, \vartheta) \end{pmatrix}, \quad (3)$$

where  $F_{nk}(r)$  and  $G_{nk}(r)$  are the radial wave functions of the upper and lower components respectively with  $Y_{jm}^l(\theta, \vartheta)$  and  $Y_{jm}^i(\theta, \vartheta)$  for spin and pseudospin spherical harmonics coupled to the angular momentum on the  $z$ -axis. Now substituting Eq. (3) into Eq. (2), we recast the following differential equations [25-28]

$$\left( \frac{d^2}{dr^2} + \frac{\kappa}{r^2} - U(r) \right) F_{nk}(r) = (M + E_{nk} - V(r) + S(r)) G_{nk}(r), \quad (4)$$

$$\left( \frac{d^2}{dr^2} - \frac{\kappa}{r^2} + U(r) \right) G_{nk}(r) = (M - E_{nk} + V(r) + S(r)) F_{nk}(r), \quad (5)$$

which later give

$$\left\{ \frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r^2} + \frac{2\kappa}{r} U(r) - \frac{dU(r)}{r} - U^2(r) + \frac{\frac{d\Delta(r)}{dr}}{M + E_{nk} - \Delta(r)} \left( \frac{d}{dr} + \frac{\kappa}{r} \right) \right\} F_{nk}(r),$$

$$= \left[ (M + E_{nk} - \Delta(r))(M - E_{nk} + \Delta(r)) \right] F_{nk}(r), \quad (6)$$

for  $\kappa(\kappa+1) = \ell(\ell+1)$ ,  $r \in (0, \infty)$ ,

$$\left\{ \frac{d^2}{dr^2} - \frac{\kappa(\kappa-1)}{r^2} + \frac{2\kappa}{r}U(r) + \frac{dU(r)}{r} - U^2(r) + \frac{\frac{d\Sigma(r)}{dr}}{M - E_{n\kappa} + \Sigma(r)} \left( \frac{d}{dr} - \frac{\kappa}{r} \right) \right\} G_{n\kappa}(r) = \left[ (M + E_{n\kappa} - \Delta(r))(M - E_{n\kappa} + \Sigma(r)) \right] G_{n\kappa}(r). \tag{7}$$

for  $\kappa(\kappa-1) = \tilde{\ell}(\tilde{\ell}+1)$ ,  $r \in (0, \infty)$ , where  $\Delta(r) = V(r) - S(r)$  and  $\Sigma(r) = V(r) + S(r)$ .

It is noted that Eqs. (6) and (7) cannot be solved for  $k \neq 0$  without the use of approximation scheme. Therefore, in this paper, we apply the following approximation-type [28].

$$\frac{1}{r^2} \approx \frac{1}{r_e^2} \left( D_0 + D_1 \frac{e^{-\alpha x}}{1 - C_h e^{-\alpha x}} + D_2 \frac{e^{-2\alpha x}}{(1 - C_h e^{-\alpha x})^2} \right), \tag{8}$$

where  $\alpha = b_h r_e$ ,  $x = \frac{r - r_e}{r_e}$ , and the parameters  $D_0$ ,  $D_1$  and  $D_2$  in the approximation are given as

$$D_0 = 1 + \frac{(1 - C_h)}{\alpha} \left[ \frac{3}{\alpha}(1 - C_h) - (3 + C_h) \right], \tag{9}$$

$$D_1 = \frac{2}{\alpha} (1 - C_h)^2 \left[ (2 + C_h) - \frac{3}{\alpha}(1 - C_h) \right], \tag{10}$$

$$D_2 = \frac{(1 - C_h)^3}{\alpha} \left[ \frac{3}{\alpha}(1 - C_h) - (1 + C_h) \right]. \tag{11}$$

### 3.0 Dirac Equation in the Presence of Shifted Tietz-Wei Potential

In this section, we obtain the solutions of Dirac equation under spin and pseudospin symmetry with shifted Tietz-Wei potential by using an elegant supersymmetric approach. For tensor term, we consider the Coulomb potential  $U(r) = -\frac{H}{r}$ .

#### 3.1 The Spin Symmetry Limit

To obtain the solution of the Dirac equation under spin symmetry limit, we take  $\frac{d\Delta(x)}{dx} = 0$  and  $\Delta(x) = C_s$ . Now, substitute potential (1) and approximation (8) into Eq. (6) to have

$$\frac{d^2 F_{n\kappa}(x)}{dx^2} = [V_{eff}^s(x) - E_{n\kappa}^s] F_{n\kappa}(x), \tag{12}$$

where

$$V_{eff}^s(x) = \frac{\left[ \left( \frac{\delta D_1}{r_e^2} (1 - C_h e^{-\alpha x}) - C_h e^{-\alpha x} \right) - 2\beta D_e \right] e^{-\alpha x} - 2\beta D_e}{1 - C_h e^{-\alpha x}} + \frac{\left[ \frac{\delta D_2}{r_e^2} + \beta D_e (C_h^2 - 2C_h - 1) \right] e^{-2\alpha x} + 2\beta D_e}{(1 - C_h e^{-\alpha x})^2}, \tag{13}$$

$$-E_{n\kappa}^s = \beta(M - E_{n\kappa}) + \frac{\delta D_0}{r_e^2}, \quad \beta = (M + E_{n\kappa} - C_s), \quad \delta = (k + H)(k + H + 1), \tag{14}$$

Here, we employ the basic concept of the supersymmetric approach [29-32] and the formula method to solve Eq. (12). The ground-state wave function for the upper component is written as

$$F_{0k}(x) = \exp\left(-\int Q(x)dx\right), \tag{15}$$

where  $Q(x)$  is called a superpotential function in supersymmetric quantum mechanics [33-36]. Substituting Eq. (15) into Eq. (12) results to the following equation satisfied by the superpotential function  $Q(x)$

$$Q^2(x) - \frac{dQ(x)}{dx} = V_{eff}^s(x) - E_{0k}^s, \tag{16}$$

where  $E_{0k}^s$  is the ground-state energy. In order to make the superpotential function  $Q(x)$  be compatible with the property of the right hand side [37, 39] of Eq. (16), we propose a superpotential function of the form

$$Q(x) = \rho_1 - \frac{\rho_2 e^{-\alpha x}}{1 - C_h e^{-\alpha x}}, \tag{17}$$

where  $\rho_1$  and  $\rho_2$  are two parametric constants to be determine later. In view of the proposed superpotential function of equation (17), we can construct a pair of supersymmetric partner potentials  $V_+(x)$  and  $V_-(x)$  in the following form:

$$V_+(x) = Q^2(x) + \frac{dQ(x)}{dx} = \rho_1^2 - \frac{2\rho_1\rho_2 e^{-\alpha x}}{1 - C_h e^{-\alpha x}} + \frac{\rho_2(\rho_2 + \alpha)e^{-\alpha x} - \rho_2^2(1 - e^{-\alpha x})e^{-\alpha x}}{(1 - C_h e^{-\alpha x})^2}, \tag{18}$$

$$V_-(x) = Q^2(x) - \frac{dQ(x)}{dx} = \rho_1^2 - \frac{2\rho_1\rho_2 e^{-\alpha x}}{1 - C_h e^{-\alpha x}} + \frac{\rho_2(\rho_2 - \alpha)e^{-\alpha x} - \rho_2^2(1 - e^{-\alpha x})e^{-\alpha x}}{(1 - C_h e^{-\alpha x})^2}. \tag{19}$$

In this work, we only consider the bound state solutions that demand the wave function  $F_{nk}(r)$  satisfying the boundary conditions:  $F_{nk}(0) = F_{nk}(\infty) = 0$ . These regularity conditions yield the restriction conditions that  $\rho_1 > 0$  and  $\rho_2 > 0$ . By substituting the superpotential function into Eq. (16) and compare the two sides of the equation, we easily deduce the values of the two parametric constants in the following form:

$$\rho_1^2 = \beta(M - E_{nk})r_e^2 + \delta D_0, \tag{20}$$

$$\rho_2 = \frac{\alpha}{2} \left[ 1 \pm \sqrt{1 + \frac{4\delta D_2 + 4\beta D_e r_e^2 (1 - C_h)^2}{\alpha^2 C_h^2}} \right], \tag{21}$$

$$\rho_1 = \frac{\beta D_e \left( 1 - \frac{1}{C_h^2} \right) + \frac{\delta}{C_h^2} (D_1 C_h - D_2) + \rho_2^2}{2\rho_2}. \tag{22}$$

With the help of the two partner potentials given in Eqs. (18) and (19), we can now write the following relationship satisfied by the shape invariance condition

$$V_+(x, a_0) = V_-(x, a_1) + R(a_1), \tag{23}$$

where  $a_1$  is a new parameter uniquely determine from an old parameter  $a_0$  and  $a_0$  is a function of  $a_1$ , i.e.  $a_1 = f(a_0) = a_0 - \alpha$ . The residual term  $R(a_1)$  is independent of the variable  $x$  However, Eqs. (18), (19) and (23) show that the partner potentials are shape invariant. By using the shape invariant approach [35], we can determine exactly, the energy eigenvalues equation of the shape invariant potential  $V_-(x)$  as we obtain the following equations

$$R(a_1) = \left[ \frac{a_0^2 + \frac{\delta}{C_h^2} (D_1 C_h - D_2) + \beta D_e \left( 1 - \frac{1}{C_h^2} \right)}{2a_0} \right]^2 - \left[ \frac{a_1^2 + \frac{\delta}{C_h^2} (D_1 C_h - D_2) + \beta D_e \left( 1 - \frac{1}{C_h^2} \right)}{2a_1} \right]^2, \tag{24}$$

$$R(a_2) = \left[ \frac{a_1^2 + \frac{\delta}{C_h^2} (D_1 C_h - D_2) + \beta D_e \left( 1 - \frac{1}{C_h^2} \right)}{2a_1} \right]^2 - \left[ \frac{a_2^2 + \frac{\delta}{C_h^2} (D_1 C_h - D_2) + \beta D_e \left( 1 - \frac{1}{C_h^2} \right)}{2a_2} \right]^2, \tag{25}$$

$$R(a_n) = \left[ \frac{a_{n-1}^2 + \frac{\delta}{C_h^2} (D_1 C_h - D_2) + \beta D_e \left(1 - \frac{1}{C_h^2}\right)}{2a_{n-1}} \right]^2 - \left[ \frac{a_n^2 + \frac{\delta}{C_h^2} (D_1 C_h - D_2) + \beta D_e \left(1 - \frac{1}{C_h^2}\right)}{2a_n} \right]^2 \quad (26)$$

Following the formalism of shape invariance approach, the energy levels of the system can be determine as

$$E_{nk}^s = E_{nk}^{s(-)} + E_{0k}^s = \sum_{i=1}^n R(a_i) + E_{0k}^s = \left[ \frac{a_n^2 + \frac{\delta}{C_h^2} (D_1 C_h - D_2) + \beta D_e \left(1 - \frac{1}{C_h^2}\right)}{2a_n} \right]^2 \quad (27)$$

$$E_{0k}^s = 0. \quad (28)$$

This gives energy equation for the spin symmetry as

$$\left( -E_{s,nk}^{s2} + M^2 \right) r_e^2 + C_s (E_{nk} - M) r_e^2 + \delta D_0 = \alpha^2 \left[ \frac{\frac{\delta(D_1 C_h - D_2)}{\alpha^2 C_h^2} + \frac{D_e r_e^2 (M + E_{nk} - C_s)}{\alpha^2 C_h^2} + \left( n + \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4[\delta D_2 + D_e b^2 r_e^2 (1 - C_h)^2 (M + E_{nk} - C_s)]}{\alpha^2 C_h^2}} \right)^2}{2n+1 + \sqrt{1 + \frac{4[\delta D_2 + D_e b^2 r_e^2 (1 - C_h)^2 (M + E_{nk} - C_s)]}{\alpha^2 C_h^2}}} \right]^2 \quad (29)$$

In other to compute the corresponding wave function using Formula method, we write a differential equation of the form [39]

$$\frac{d^2 F_{nk}(z)}{dz^2} + \frac{\alpha_1 - \alpha_2 z}{s(1 - \alpha_3 z)} \frac{dF_{nk}(z)}{dz} + \left[ \frac{A_2 z^2 + A_1 z + A_0}{(z(1 - \alpha_3 z))^2} \right] F_{nk}(z), \quad (30)$$

the wave function is given as [39]

$$F(z) = N_n z^\varepsilon (1 - \alpha_3 z)^\varsigma {}_2P_1 \left( -n, n + 2(\varepsilon + \varsigma) + \frac{\alpha_2}{\alpha_3} - 1; 2\varepsilon + \alpha_1, \alpha_3 z \right), \quad (31)$$

$$\varsigma = \frac{1}{2} + \frac{\alpha_1}{2} - \frac{\alpha_2}{2\alpha_3} + \sqrt{\left( \frac{1}{2} + \frac{\alpha_1}{2} - \frac{\alpha_2}{2\alpha_3} \right)^2 - \left( \frac{A_2}{\alpha_3 \alpha_3} + \frac{A_1}{\alpha_3} + A_0 \right)}, \quad \varepsilon = \frac{(1 - \alpha_1) + \sqrt{(1 - \alpha_1)^2 - 4A_{1=0}}}{2}.$$

Defining a variable of the form  $s = C_h e^{-\alpha x}$  and substitute it into Eq. (12), we have the following

$$\frac{d^2 F_{nk}(s)}{ds^2} + \frac{1-s}{s(1-s)} \frac{dF_{nk}(s)}{ds} + \left[ \frac{B_2 s^2 + B_1 s + B_0}{(s(1-s))^2} \right] F_{nk}(s), \quad (32)$$

where

$$B_2 = 1 + \frac{4}{r_e^2} \left[ \delta \left( \frac{D_2}{C_h^2} + D_0 - D_1 \right) + 2\beta D_e C_h^2 \left( C_h + \frac{1}{C_h^2} - 1 \right) \right], \quad (33)$$

$$B_1 = \frac{2}{C_h^2} \left[ 2\beta (D_e - M + E_{nk}) r_e^2 + \delta D_0 \right], \quad (34)$$

$$B_0 = \beta (M - E_{nk}) - 2\beta D_e C_h - \frac{\delta D_0}{r_e^2}. \quad (35)$$

Thus, the upper component of the wave function is written as

$$F(s) = N_n s^\varepsilon (1-s)^\zeta {}_2P_1(-n, n+2(\varepsilon+\zeta); 2\varepsilon+1, s), \quad (36)$$

### 3.2 Pseudospin Symmetry Limit

To obtain the solution of the Dirac equation under pseudospin symmetry limit, we take  $\frac{d\Sigma(x)}{dx} = 0$  and  $\Sigma(x) = C_{ps}$ , we substitute potential (1) and approximation (8) into Eq. (7) to have

$$\frac{d^2 G_{nk}(x)}{dx^2} = [V_{eff}^{ps}(x) - E_{nk}^{ps}] F_{nk}(x), \quad (37)$$

where

$$V_{eff}^{ps}(x) = \frac{\left[ \left[ \frac{\delta_1 D_1}{r_e^2} (1 - C_h e^{-\alpha x}) - C_h e^{-\alpha x} \right] + 2\beta_1 D_e \right] e^{-\alpha x} + 2\beta_1 D_e}{1 - C_h e^{-\alpha x}} + \frac{\left[ \frac{\delta_1 D_2}{r_e^2} + \beta_1 D_e (C_h^2 - 2C_h - 1) \right] e^{-2\alpha x} - 2\beta_1 D_e}{(1 - C_h e^{-\alpha x})^2}, \quad (38)$$

$$-E_{nk}^{ps} = \beta_1 (M + E_{nk}) + \frac{\delta_1 D_0}{r_e^2}, \quad \beta_1 = (M - E_{nk} + C_{ps}), \quad \delta_1 = (k + H)(k + H - 1) \quad (39)$$

The negative energy solution of Eq. (6) can directly be obtained via the spin symmetry solution through the mapping

$$F_{nk}(x) \leftrightarrow G_{nk}(x), -E_{nk} \rightarrow E_{nk}, V(r) \rightarrow -V(r), -C_s \rightarrow C_{ps}, k \rightarrow k - 1, \quad (40)$$

Following the previous steps and methodologies, we obtain the energy equation for the pseudospin symmetry as

$$\left( -E_{ps,nk}^2 + M^2 \right) r_e^2 - C_{ps} (E_{nk} - M) r_e^2 + \delta_1 D_0 = \frac{\left[ \frac{\delta_1 (D_1 C_h - D_2)}{\alpha^2 C_h^2} - \frac{D_e r_e^2 (M - E_{nk} + C_{ps}) \left( 1 - \frac{1}{C_h} \right)}{\alpha^2 C_h^2} + \left( n + \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4 \left[ \delta_1 D_2 r_e^2 - D_e b^2 r_e^2 (1 - C_h)^2 (M - E_{nk} + C_{ps}) \right]}{\alpha^2 C_h^2}} \right)^2 \right]^2}{2n + 1 + \sqrt{1 + \frac{4 \left[ \delta_1 D_2 r_e^2 - D_e b^2 r_e^2 (1 - C_h)^2 (M - E_{nk} + C_{ps}) \right]}{\alpha^2 C_h^2}}}. \quad (41)$$

and the corresponding lower component wave function is

$$G(s) = N_n s^{\varepsilon_1} (1-s)^{\zeta_1} {}_2P_1(-n, n+2(\varepsilon_1+\zeta_1); 2\varepsilon_1+1, s), \quad (42)$$

### 3.3 Non-Relativistic Limit

In this section, we obtain the non-relativistic limit of the spin symmetry limit. The non-relativistic Schrödinger equation is bosonic in nature, i.e., spin does not involve in it. On the other hand, relativistic Dirac equation is for a spin-1/2 particle. It implicitly suggests that there may be a certain relation between the solutions of the two fundamental equations [40-42]. That is, the non-relativistic energies  $E_{NR}$  can be determined by taking the non-relativistic limit values of the relativistic eigenenergies  $E$ .

Therefore, taking  $C_s = H = 0$ , and using the transformations  $M + E_{nk} \rightarrow \frac{2\mu}{\hbar^2}$  and  $M - E_{nk} \rightarrow -E_{n\ell}$

together with  $\kappa \rightarrow \ell$  [42], the relativistic energy Eq. (29) reduces to

$$E_{n\ell} = \frac{\alpha^2 \hbar^2}{2\mu} \frac{\ell(\ell+1) D_0}{\alpha^2 r_e^2} \left[ \frac{\left( \frac{\ell(\ell+1)(D_1 C_h - D_2)}{\alpha^2 C_h^2} + \frac{2\mu D_e r_e^2 \left( 1 - \frac{1}{C_h} \right)}{\alpha^2 \hbar^2} + \left[ n + \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4\ell(\ell+1)D_2 + 8\mu D_e r_e^2 (1 - C_h)^2}{\alpha^2 C_h^2 + \alpha^2 \hbar^2 C_h^2}} \right]^2 \right)^2}{2n + 1 + \sqrt{1 + \frac{4\ell(\ell+1)D_2 + 8\mu D_e r_e^2 (1 - C_h)^2}{\alpha^2 C_h^2 + \alpha^2 \hbar^2 C_h^2}}} \right]. \quad (43)$$

Eq. (43) is identical to equation (16) of Ref. [24]. The corresponding wave function is given as

$$R_{n\ell}(s) = N_{n\ell} s^a (1-s)^b {}_2F_1(-n, n+2(a+b); 2a+1, s), \quad (44)$$

where,

$$a = \sqrt{\frac{\ell(\ell+1)D_0}{\alpha^2} - \frac{2\mu r_e^2 E_{n\ell}}{\alpha^2 \hbar^2}} \quad \text{and} \quad b = \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4\ell(\ell+1)D_2}{\alpha^2 C_h^2} + \frac{8\mu D_e r_e^2 (1-C_h)^2}{\alpha^2 \hbar^2 C_h^2}}.$$

#### 4.0 Thermodynamic Properties and the Shifted Tietz-Wei Potential

In order to calculate the thermodynamic properties of a system within the Shifted Tietz-Wei diatomic potential model, we first calculate the vibrational partition function of the system. To begin, we first re-write the energy equation (43) in the form:

$$E_{n,\ell} = \frac{\ell(\ell+1)\delta^2 \hbar^2}{2\mu r_e^2} - \frac{\delta^2 \hbar^2}{2\mu} \left[ \frac{\xi + (\lambda + n)^2}{2(\lambda + n)} \right]^2. \quad (45)$$

where

$$\xi = \frac{\ell(\ell+1)(D_1 C_h - D_2)}{\alpha^2 C_h^2} + \frac{2\mu D_e r_e^2 \left(1 - \frac{1}{C_h^2}\right)}{\alpha^2 \hbar^2} \quad \lambda = \frac{1}{2} + \frac{1}{2} \sqrt{1 + \frac{4\ell(\ell+1)D_2}{\alpha^2 C_h^2} + \frac{8\mu D_e r_e^2 (1-C_h)^2}{\alpha^2 \hbar^2 C_h^2}} \quad \text{and } [\lambda] \text{ means}$$

the largest integer inferior to  $\lambda$ . Now, the partition function of the system is calculated by

$$Z(\beta) = \sum_{n=0}^{\lambda} e^{-\beta E_{n\ell}}, \quad \beta = \frac{1}{kT}. \quad (46)$$

Substituting Eq. (39) into Eq. (40), we have

$$Z(\beta) = e^{-\beta \left( \frac{\ell(\ell+1)D_0 \alpha^2 \hbar^2}{2\mu r_e^2} \right)} \sum_{n=0}^{\lambda} e^{\left[ \frac{\xi + (\lambda+n)^2}{2(\lambda+n)} \right]^2}, \quad \mathfrak{R} = \frac{\gamma}{\sqrt{\beta}}, \quad \gamma = \frac{r_e \sqrt{2\mu}}{\alpha \hbar}. \quad (47)$$

In the classical limit at high temperature T, for large  $\lambda$  and small  $\beta$ ,  $e^{-\beta \left( \frac{\ell(\ell+1)D_0 \alpha^2 \hbar^2}{2\mu r_e^2} \right)} \approx 1$ , the sum can be replaced by the integral to have the partition function as

$$Z(\beta) = \mathfrak{R} \int_0^{\lambda} e^{z^2} dz = \frac{\sqrt{\pi} \gamma \operatorname{Erfi} \left( \frac{\lambda}{\gamma} \sqrt{\beta} \right)}{\beta}, \quad z = \frac{\xi + (\lambda+n)}{2(\lambda+n)}. \quad (48)$$

Having obtained the partition function in Eq. (48), it becomes less cumbersome to calculate the thermodynamic properties.

#### 4.1 The Vibrational Mean Energy U

$$\begin{aligned} U(\beta) &= -\frac{\partial}{\partial \beta} \ln Z(\beta) = \frac{1}{\beta} \left[ 1 - \frac{\tau}{\operatorname{DawsonF}(\tau)} \right] \\ &= \frac{-\tau}{\sqrt{\pi} \operatorname{Erfi}(\tau)} \left[ \frac{e^\tau}{\beta} - \frac{\sqrt{\pi} \operatorname{Erfi}(\tau)}{2\beta\tau} \right], \quad \tau = \tau(\beta) = \frac{\lambda}{\gamma} \sqrt{\beta}. \end{aligned} \quad (49)$$

#### 4.2 The Vibrational Specific Heat C

$$C(\beta) = \frac{\partial}{\partial T} U(\beta) = k\beta^2 \frac{\partial}{\partial \beta} U(\beta)$$

$$= \frac{1}{2}k \left[ 1 - \frac{\tau \left[ \tau e^{\tau^2} + \sqrt{\pi}(1-\tau^2) \operatorname{Erfi}(\tau) \right]}{2e^{\tau^2} \operatorname{DawsonF}(\tau)^2} \right], \tag{50}$$

When  $\beta \ll 1$ ,  $C(\beta) = 0$ .

### 4.3 The Vibrational Mean Free Energy F

$$F(\beta) = -kT \ln Z(\beta) = -\frac{1}{\beta} \ln \left( \frac{\sqrt{\pi} \gamma \operatorname{Erfi}(\tau)}{\sqrt{\beta}} \right). \tag{51}$$

#### 4.4: The Vibrational Entropy S:

$$S(\beta) = k \ln Z(\beta) + kT \frac{\partial}{\partial \beta} \ln Z(\beta) = S(\beta) = k \ln Z(\beta) - k\beta \frac{\partial}{\partial \beta} \ln Z(\beta)$$

$$\frac{1}{2}k \left[ 1 - \frac{\tau}{\operatorname{DawsonF}(\lambda)} + 2 \log \left( \frac{\gamma \operatorname{Erfi}(\tau)}{\frac{1}{2} \sqrt{\beta}} \right) + \log \left( \frac{\pi}{2} \right) \right]. \tag{52}$$

### 5.0 Information Entropy

In this section, we consider the information entropy of the Shifted Tietz-Wei potential. Entropy is the key concept of quantum information theory. It measures how much uncertainty present in a state of a physical system. In the context of this work, we consider the Shannon entropy, the Renyi entropy and Onicescu energy.

#### 5.1 Shannon Entropy

In the position space, the Shannon information entropy  $S_\rho$  of an electron density  $\rho(x)$  in the coordinate space is defined as [43-45]

$$S(\rho) = -4\pi \int \rho(x) \ln \rho(x) dx, \tag{53}$$

where

$$\rho(x) = N_{nl}^2 s^{2a} (1-s)^{2b} \times {}_2F_1(-n, n+2(a+b); 2a+1; s)^2, \tag{54}$$

where we have defined a variable of the form  $s = e^{-\alpha x}$  and  $C_h = 1$ . Substituting Eq. (54) into Eq. (53), we have

$$S(\rho) = \frac{4\pi N_{nl}^2}{\alpha s} \ln \rho(s) \int_1^0 s^{2a} (1-s)^{2b} {}_2F_1(-n, n+2(a+b); 2a+1; s)^2 ds, \tag{55}$$

$$S(\rho) = \frac{-4\pi N_{nl}^2}{\alpha(1-y)} \ln \rho(y) \int_0^1 y^{2b} (1-y)^{2a} {}_2F_1(-n, n+2(a+b); 2a+1; s)^2 dy, s = 1-y, \tag{56}$$

Let us now define a function of the form

$$\int_0^1 y^{2b} (1-y)^{2a} {}_2F_1(-n, n+2(a+b); 2a+1; y)^2 dy = \frac{n! \Gamma(2a+1)^2 \Gamma(2b+n+2)}{2b \Gamma(2a+n+1) \Gamma(2a+2b+n+2)}, \tag{57a}$$

$${}_2F_1(-n, n+2(a+b); 2a+1; s) ds = \frac{\Gamma(2a+1) \Gamma(1-2b)}{\Gamma(2a+n+1) \Gamma(1-n-2b)}. \tag{57b}$$

Using Eqs. (57), the Shannon entropy in the position space is obtained as

$$S(\rho) = -\frac{12.568}{\alpha(1-z)} \ln \left[ 2bm(1-y)^{2b} \frac{\Gamma(2a+n+1) \Gamma(2a+2b+n+2)}{n! \Gamma(2a+1)^2 \Gamma(2b+n+2)} \left( \frac{\Gamma(2b+1) \Gamma(1-2a)}{\Gamma(2b+n+1) \Gamma(1-n-2a)} \right)^2 \right]. \tag{58}$$



In the momentum space, the Shannon information entropy is [45]

$$S_{[\gamma]} = -4\pi \int_0^\infty \gamma(p) \ln \gamma(p) dp, \tag{59}$$

where

$$\gamma(p) = N_{nl}^2 e^{-2ab_h(p-r_e)} \left(1 - C_h e^{-b_h(p-r_e)}\right)^{2b} \left[ P_n^{(2a, 2b-1)} \left(1 - 2C_h e^{-b_h(p-r_e)}\right) \right]^2. \tag{60}$$

Eq. (58) is equal to Eq. (54). Defining  $z = e^{-b_h(p-r_e)}$ . Thus, Eq. (59) becomes

$$S_{[\gamma]} = 4\pi\beta_1 \bar{D} N_{nl}^2 \int_0^1 y^{2a} (1-y)^{2b} dy, \quad z = 1-y, \tag{61}$$

where  $\beta_1 = \left[ P_n^{(2a, 2b-1)} (2y-1) \right]^2 (1-y)^{-1}$  and  $\bar{D} = \ln \gamma(p)$ .

Following two different forms of Jacobi polynomials [46, 47]

$$P_n^{(\alpha, \beta)}(s) = \frac{\Gamma(\alpha+n+1)}{n! \Gamma(\alpha+\beta+n+1)} \times \sum_{m=0}^n \binom{n}{m} \frac{\Gamma(\alpha+\beta+n+m+1)}{\Gamma(\alpha+m+1)} \left(\frac{s-1}{2}\right)^m, \tag{62}$$

$$P_n^{(\alpha, \beta)}(s) = \frac{1}{2^n} \sum_{k=0}^n \binom{n+\alpha}{k} \binom{n+\beta}{k} \times \binom{n+\beta}{n-k} (s-1)^{n-k} (s+1)^k, \tag{63}$$

and the integral of appendix (A.3), we deduce the momentum space Shannon entropy as follows:

$$S_{[\gamma]} = \left[ \begin{aligned} & \frac{12.568 N_{nl}^2}{1-y} \frac{\Gamma(2a+n+1)}{n! \Gamma(2a+2b+n)} \times \frac{1}{2^n} \sum_{m=0}^n \sum_{k=0}^n \binom{n}{m} \frac{\Gamma(2a+2b+n+m+1)}{\Gamma(\alpha+m+1)} (y-1)^m \\ & \left( \binom{n+2a}{k} \binom{n+2b-1}{k} \times \binom{n+2b-1}{n-k} \right) (2(y-1))^{n-k} (2y)^k \left( \frac{1}{1+2a} {}_2F_1(-2b, 1+2a, 2(1+a); 1) \right) \\ & \ln \left[ N_{nl}^2 y^{2a} (1-y)^{2b+1} \beta_1 \right] \end{aligned} \right], \tag{64}$$

### 5.2 The Renyi Entropy

The Renyi entropy in position space is defined as [48, 49]

$$R_q[\rho] = \frac{1}{1-q} \log \left[ \int \rho(x)^q dx \right], \quad 0 < q < \infty, \quad q \neq 1. \tag{65}$$

Substituting Eq. (60) into Eq. (65), the Renyi entropy is obtain as

$$R_q[\rho] = \frac{1}{1-q} \log \left[ \frac{\left( N_{nl}^2 \left(\frac{1-t}{2}\right)^{2a} \left(\frac{1+t}{2}\right)^{2b} \times \left[ P_n^{(2a, 2b-1)}(t) \right]^2 \right)^{q-1}}{1+q} \right]. \tag{66}$$

The momentum space is define as

$$R_q[\gamma] = \frac{1}{1-q} \log \left[ 4\pi \int_0^\infty \gamma(p)^q dp \right], \quad 0 < q < \infty, \quad q \neq 1. \tag{67}$$

Substitute Eq. (60) into Eq. (67) we obtain the momentum space for the Renyi entropy as

$$R_q[\gamma] = \frac{1}{1-q} \log \left[ 12.568 N_{nl}^{2q} \times \frac{\left( \frac{1}{1+2a} {}_2F_1(-2b, 1+2a, 2(1+a); 1) \right)^q \frac{\Gamma(2a+n+1)}{n! \Gamma(2a+2b+n)}}{\frac{1}{2^n} \sum_{m=0}^n \sum_{k=0}^n \binom{n}{m} \frac{\Gamma(2a+2b+n+m+1)}{\Gamma(\alpha+m+1)} (y-1)^m} \left( \binom{n+2a}{k} \binom{n+2b-1}{k} \times \binom{n+2b-1}{n-k} \right) (2(y-1))^{n-k} (2y)^k \right]. \tag{68}$$

### 5.3 The Onicescu Information Energy

The Onicescu information energy is defined as [50]

$$E[\rho] = \int \rho(x)^2 dx. \tag{69}$$

Recall that  $\alpha = b_h r_e$ ,  $x = \left(\frac{r-r_e}{r_e}\right)$  and consider  $s = e^{-b_h(r-r_e)}$ , Eq. (69) can be written as

$$E[\rho] = \int_0^\infty \rho(x)^2 dx = \int_0^{C_h e^{b_h r_e}} \rho^2(s) \frac{1}{b_h s} ds. \tag{70}$$

Because of the cumbersome nature and difficulty in calculating Eq. (70) due to the interval of the variable  $[0, C_h e^{b_h r_e}]$  [51, 52], Wei weakening the limit of the integral [53] from  $[0, C_h e^{b_h r_e}]$  to  $[0, 1]$ . Now, recall that  $t = 1 - 2s$ , Eq. (62) becomes

$$E[\rho] = \frac{1}{2b_h} \int_{-1}^1 \rho^2(t) \frac{2}{1-t} dt. \tag{71}$$

Substituting for  $\rho(t)$  into Eq. (71), we obtain the Onicescu information energy as

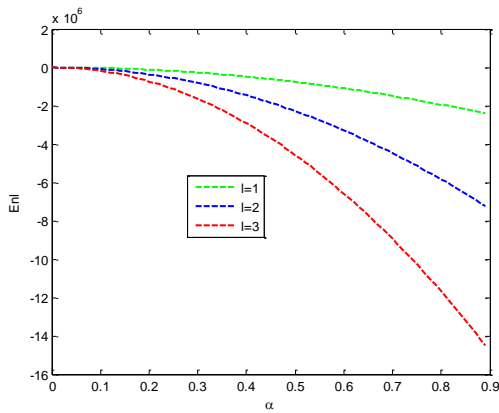
$$E[\rho] = b_h^2 \left( N_{nt}^2 \right)^2 \left[ \begin{aligned} & (b+1) \frac{2\Gamma(2a+n+1)\Gamma(2b+n+1)}{n!2a\Gamma(2(a+b+n+1))\Gamma(2a+2b+n+1)} + \\ & a \frac{2\Gamma(2a+n+1)\Gamma(2b+n+2)}{n!2a\Gamma(2(a+b+n+1))\Gamma(2a+2b+n+2)} + \\ & 2 \frac{\Gamma(2a+n+1)\Gamma(2b+n+2)}{n!2a\Gamma(2(a+b+1)+n)\Gamma(2a+2b+n+1)} \end{aligned} \right]. \tag{72}$$

**Table 1:** Bound states for the spin symmetry limit in units of  $fm^{-1}$  ( $E_{s,n,\kappa}(fm^{-1})$ ) for  $D_e = 38$ ,  $b_h = 1.6189$ ,  $C_h = 0.170066$ ,  $M = b_h - 2C_h$ ,  $r_e = 0.7416$ ,  $C_s = 5fm^{-1}$ .

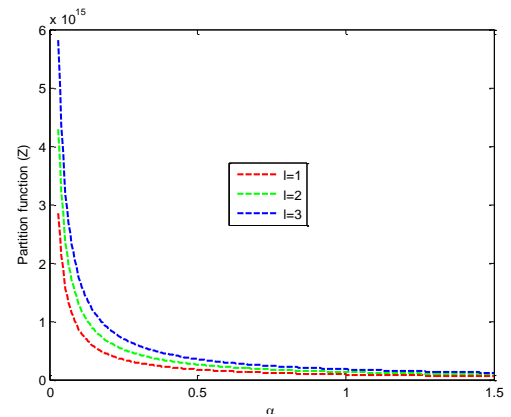
$(l, j)$	$H = 0$	$(l, j)$	$H = 0.5$	$(l, j)$	$H = 1$
$0p_{3/2}, 0p_{1/2}$	3.721311056	$0d_{5/2}, 0p_{3/2}$	3.721464804	$0s_{1/2}, 0p_{3/2}$	3.721310321
$0d_{5/2}, 0d_{3/2}$	3.721001774	$1d_{5/2}, 1p_{3/2}$	3.721034969	$1s_{1/2}, 1p_{3/2}$	3.721045463
$0f_{7/2}, 0f_{5/2}$	3.720711285	$2d_{5/2}, 2p_{3/2}$	3.720622920	$2s_{1/2}, 2p_{3/2}$	3.720176882
$1p_{3/2}, 1p_{1/2}$	3.720069537	$3d_{5/2}, 3p_{1/2}$	3.720230477	$3s_{1/2}, 3p_{3/2}$	3.720067321
$1d_{5/2}, 1d_{3/2}$	3.721680719	$0f_{7/2}, 0d_{3/2}$	3.721958249	$0f_{7/2}, 0p_{1/2}$	3.721680071
$1f_{7/2}, 1f_{5/2}$	3.721132608	$1f_{7/2}, 1d_{3/2}$	3.721292950	$1f_{7/2}, 1p_{1/2}$	3.721132608
$2p_{3/2}, 2p_{1/2}$	3.720260716	$2f_{7/2}, 2d_{3/2}$	3.720644498	$2f_{7/2}, 2p_{1/2}$	3.720601714
$2d_{5/2}, 2d_{3/2}$	3.720089470	$3f_{7/2}, 3d_{3/2}$	3.720014080	$3f_{7/2}, 3p_{1/2}$	3.722008947
$2f_{7/2}, 2f_{5/2}$	3.722297166				
$3p_{3/2}, 3p_{1/2}$	3.721515288				
$3d_{5/2}, 3d_{3/2}$	3.720749997				
$3f_{7/2}, 3f_{5/2}$	3.720002305				

**Table 2:** Bound states for the pseudospin symmetry limit in units of  $fm^{-1} (E_{s,n,\kappa}(fm^{-1}))$  for  $D_e = 38$ ,  $b_h = 1.6189$ ,  $C_h = 0.170066$ ,  $M = b_h - 2C_h$ ,  $r_e = 0.7416$ ,  $C_{ps} = 5fm^{-1}$ .

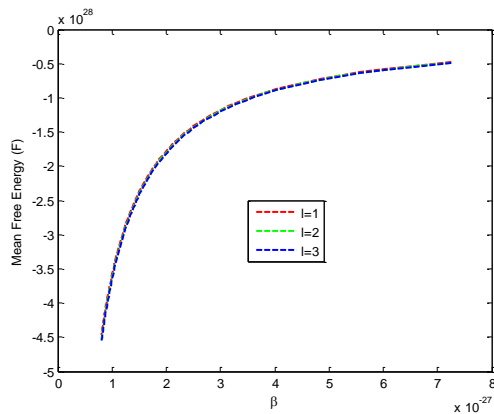
$(l, j)$	$H = 0$	$(l, j)$	$H = 0.5$	$(l, j)$	$H = 1$
$1s_{1/2}, 0d_{3/2}$	-3.284208061	$1p_{3/2}, 0d_{3/2}$	-3.291353680	$1d_{5/2}, 0d_{3/2}$	-3.299592716
$1p_{3/2}, 0f_{5/2}$	-3.299592716	$1d_{5/2}, 0f_{5/2}$	-3.309301496	$1f_{7/2}, 0f_{5/2}$	-3.320552256
$1d_{5/2}, 0g_{7/2}$	-3.320552256	$1f_{7/2}, 0g_{7/2}$	-3.333374313	$2d_{5/2}, 1d_{3/2}$	-3.302703958
$1f_{7/2}, 0h_{9/2}$	-3.347785341	$2p_{3/2}, 1d_{3/2}$	-3.293771766	$2f_{7/2}, 1f_{5/2}$	-3.324983346
$2s_{1/2}, 1d_{3/2}$	-3.285840469	$2d_{5/2}, 1f_{5/2}$	-3.313078666		
$2p_{3/2}, 1f_{5/2}$	-3.302703958	$2f_{7/2}, 1g_{7/2}$	-3.338453473		
$2d_{5/2}, 1g_{7/2}$	-3.324983346				
$2f_{7/2}, 1h_{9/2}$	-3.353509891				



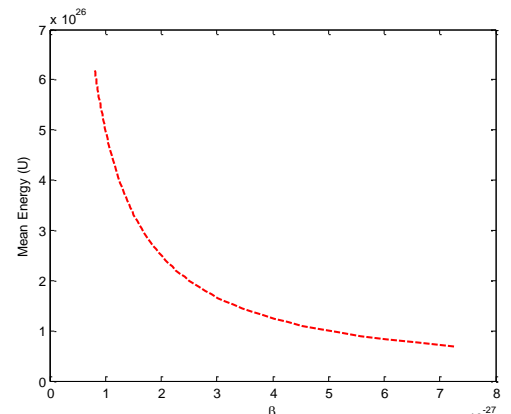
**Fig. 1:** Energy ( $E_{nl}$ ) against  $\alpha$  with  $\mu = \hbar = 1$ ,  $r_e = 0.2$ ,  $C_h = 1$ ,  $D_e = 10$ ,  $D_0 = 1$ ,  $D_1 = -D_0$  and  $D_2 = 2D_0$ .



**Fig. 2:** Variation of partition function ( $Z$ ) with  $\alpha$ .



**Fig. 3:** Variation of Mean Free energy ( $F$ ) with  $\beta$ .



**Fig. 4:** Variation of Mean energy ( $U$ ) with  $\beta$ .

## 6.0 Discussion and Results

In Tables 1 and 2, we present the numerical results for the spin symmetry and pseudospin symmetry respectively. There are degeneracies in both the spin and pseudospin symmetries. The presence of the tensor potential removes the degeneracies.

In Fig. 1, we plotted energy against  $\alpha$  for  $\ell = 1, 2, 3$ . It is found that the energy increases towards negative direction with increasing  $\ell$  when  $\alpha > 0.1$ . In Fig. 2, we observe the variation of the partition function with  $\alpha$ . It is observed that as  $\alpha$  increases, the partition function ( $Z$ ) tends towards zero. In Fig. 3 and 4, we plotted the Mean Free energy (F) and Mean energy (U) respectively with  $\beta$ . It is found that the Mean Free energy increases as  $\beta$  increases but the Mean energy decreases as  $\beta$  increases. This indicates that at higher temperature, a particle confining within a system of Shifted Tietz-Wei potential has more Mean energy than Mean Free energy.

## 7.0 Conclusion

In this paper, we have investigated the bound state solutions of the Dirac equation under spin and pseudospin symmetry limits with Shifted Tietz-Wei potential for any spin-orbit quantum number  $k$ . By using a suitable approximation scheme, we have obtained energy equations and the radial wave functions. The thermodynamic properties and information entropy of the Shifted Tietz-Wei potential have been studied. It is seen that the present result agrees with the previous results obtained in [26]. Our results found its application in atomic and molecular physics.

### Appendix A. Some useful standard integrals.

$$\int x^n dx = \frac{1}{n+1} x^{n+1}. \quad \text{A.1}$$

$$\int x \ln x dx = \frac{1}{2} x^2 \ln x - \frac{x^2}{4}. \quad \text{A.2}$$

$$\int_0^w z^y (1-pz)^t dz = \frac{w^{1+y}}{1+y} {}_2F_1(-t, 1+y, 2+y; pw). \quad \text{A.3}$$

$$\int_{-1}^1 \left(\frac{1-x}{2}\right)^a \left(\frac{1+x}{2}\right)^b \times [P_n^{(a,b)}(x)]^2 = \frac{2\Gamma(a+n+1)\Gamma(b+n+1)}{n!a\Gamma(a+b+2n+1)\Gamma(a+b+n+1)}. \quad \text{A.4}$$

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