The $^3S_1$ and $^3D_1$ n-p scattering phase shifts using semiclassical wave equations

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A semiclassical treatment is developed for n-p scattering leading to decoupled equations (to order $O(\hbar^2)$) even in the presence of tensor interaction. as the orbital angular momentum is not conserved with the tensor interaction the triplet states with the same angular momentum J have two orbital angular momenta. For example, coupling the total spin $S = 1$ with two orbital angular momenta $L = 0$ and $L = 2$ produce a state with $J = 1$ and same positive parity. The second order differential equations coupling the $^3S_1$ state, $u(r)$ and $^3D_1$ state, $w(r)$ for the n-p scattering are

$$-\frac{\hbar^2}{M}\frac{d^2u}{dr^2} + V_c(r)u - Eu = -\sqrt{8}V_t(r)w \quad (1)$$

$$-\frac{\hbar^2}{M}\left(\frac{d^2w}{dr^2} - \frac{6w}{r^2}\right) + [V_c(r) - 2V_t(r)]w - Ew = -\sqrt{8}V_t(r)u \quad (2)$$

where M is the reduced mass of the n-p scattering state, $V_c(r)$ and $V_T(r)$ are the central and tensor parts of the n-p interaction. For the Reid soft core potential, we can write

$$V(r) = V_c + V_tS_{12} + V_{LS}(\mathbf{L}.\mathbf{S}) \quad (3)$$

with

$$V_c(r) = -10.463e_1(x) + 105.468e_2(x) - 3187.8e_4(x) + 9924.3e_6(x), \quad (4)$$

$$V_t(r) = -10.463\left[\left(1 + \frac{3}{x} + \frac{3}{x^2}\right)e_1(x) - \left(\frac{12}{x} + \frac{3}{x^2}\right)e_4(x)\right] + 351.77e_4(x) - 1673.5e_6(x), \quad (5)$$

$$V_{LS} = 708.91e_4(x) - 2713.1e_6(x)$$

where $e_n(x) = e^{-nx}/x$ and $x = 0.7r$. Writing Eqs.(1) and (2) in a matrix eigenvalue form,

$$\mathbf{H}\Psi = E\Psi \quad (6)$$

with

$$\Psi = \begin{bmatrix} u \\ w \end{bmatrix},$$

$$\mathbf{H} = \left(\frac{-\hbar^2}{M}\frac{d^2}{dr^2}\right)\mathbf{I} + \mathbf{V}(r),$$

$$\mathbf{V}(r) = \begin{bmatrix} V_c(r) & \sqrt{8}V_t(r) \\ \sqrt{8}V_t(r) & \frac{6\hbar^2}{Mr^2} + V_c(r) - 2V_t(r) \end{bmatrix} \quad (7)$$

Here, $\mathbf{I}$ is an identity matrix. Potential matrix $\mathbf{V}$ being real-symmetric, the diagonalizing transformation is orthogonal $\mathbf{O}$, such that

$$\mathbf{O}(r)^T\mathbf{V}(r)\mathbf{O}(r) = \mathbf{v}(r) = \begin{bmatrix} v_+(r) & 0 \\ 0 & v_-(r) \end{bmatrix},$$

$$\text{where } \mathbf{O}(r) = \begin{bmatrix} \cos\theta/2 & \sin\theta/2 \\ -\sin\theta/2 & \cos\theta/2 \end{bmatrix},$$

$$\text{with } \tan\theta = \frac{\sqrt{8}V_t(r)}{\frac{3\hbar^2}{Mr^2} - V_t(r)} \quad (8)$$

$$v_\pm(r) = a(r) \pm b(r)\cos\theta(r) \mp \sqrt{8}V_t(r)\sin\theta(r)$$

where $a(r) = \frac{3\hbar^2}{Mr^2} + V_c(r) - V_t(r)$ and $b(r) = -\frac{3\hbar^2}{Mr^2} + V_t(r)$.

Since $-i\hbar\frac{d}{dr}(= p_r)$ does not commute with r, there appears a vector potential $\mathbf{A}$ but we note that it is purely off-diagonal and carries an order of $\hbar$ with it. We take only terms of order $O(\hbar^0)$ and take the similarity-transformed Hamiltonian, $\mathbf{H}^{(1)} = \mathbf{O}^T\mathbf{H}\mathbf{O}$ to get diagonalized form of the Hamiltonian as $\mathbf{H}_{\mu\nu} = h^\mu\delta_{\mu\nu}$ where

$$h^{(\pm)} = \left(-\frac{\hbar^2}{M}\right)\left[1 \pm \frac{\hbar^2}{M(v_+(r) - v_-(r))}\left(\frac{d\theta(r)}{dr}\right)^2\right] * \frac{d^2}{dr^2} + v_\pm(r) + \frac{\hbar^2}{8M}\left(\frac{d\theta(r)}{dr}\right)^2. \quad (9)$$

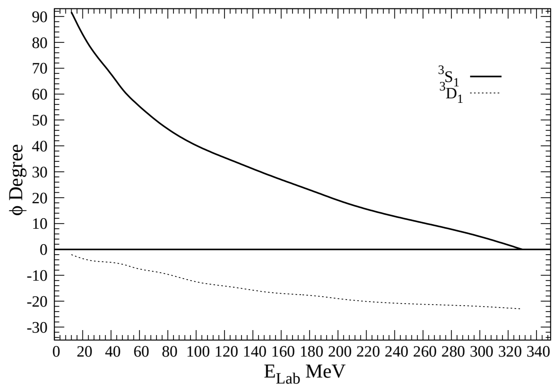

FIG. 1: Phase shifts as a function of lab energy

With this,

$$\psi^{+}(r) = u(r)\cos\frac{\theta(r)}{2} - w(r)\sin\frac{\theta(r)}{2},$$
$$\psi^{-}(r) = u(r)\sin\frac{\theta(r)}{2} + w(r)\cos\frac{\theta(r)}{2} \quad (10)$$

For large values of r, we get $\theta \sim 0$. Therefore, as $r \to \infty$,

$$\psi^{+}(r) = u(r), \quad \psi^{-}(r) = w(r). \qquad (11)$$

These equations are numrically solved using the Runga-Kutta method and matching $\psi(r)$ and their derivatives with the asymptotic scattering state wavefunctions the phase shifts are evaluated. Thus one obtains the phase shifts for $^3S_1$ and $^3D_1$ scattering states.

In Fig. **??**, the results are in good agreement with large matrix diagonalizations results. Good agreement indicates the success of our semiclassical wave equations which are quite simple and physically appealing.

References

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[2] S. R. Jain, J. Phys. G **30**, 157 (2004).