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SEMICLASSICAL AND QUANTUM MECHANICAL TREATMENTS OF POSITIVE AND NEGATIVE ANGLE POLARIZED HEAVY ION SCATTERING

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Résumé - Nous utilisons une théorie semiclassique pour calculer les sections efficaces et les pouvoirs d'analyse à tout ordre en diffusion élastique d'ions lourds polarisés. Cette approche a pour but d'expliquer les déviations par rapport à l'absence de structure observée normalement dans les sections efficaces. Ces déviations sont dues aux interférences entre diffraction et réfraction. Nous montrons que la diffusion réfractive à angle négatif ("far-side scattering") peut être interprétée comme un effet de taille de la cible à $E_{lab} \approx 20$ MeV pour ${}^6\text{Li} + {}^{12}\text{C}$. Il est montré que le très grand nombre d'intégrales à calculer numériquement limite le champ d'application de la méthode semiclassique. Finalement nous présentons une approche quantique pour traiter la diffusion à angles positifs et négatifs.

Abstract - A unified semiclassical theory for calculating cross section and analysing powers of all ranks for polarized heavy ion elastic scattering is applied to explain deviations from the structureless pattern normally encountered in the cross section, which are interpreted as due to interference between diffraction and refraction. Refractive, negative angle or far-side scattering is then discussed and is shown to be a target-size effect at $E_{lab} \approx 20$ MeV for ${}^6\text{Li} + {}^{12}\text{C}$. The limitations of the semiclassical method are then shown in terms of the necessity of performing a huge number of integrals numerically. Lastly, a quantum mechanical approach for handling positive and negative angle scattering is presented.

I - INTRODUCTION

Experimental data of polarization observables along with elastic scattering cross sections can most assuredly be expected to provide a more stringent handle on studying interference effects arising from negative angle scattering compared to the situation without analysing power measurements. This is because one would then utilise an additional degree of freedom, namely spin, over and above unpolarized cross section measurement, provided one can experimentally study effects of spin on cross section,

i.e. analysing powers. Thus a fuller set of measurements composed of analysing powers of as many ranks as possible for the same scattering process would provide a ground for testing the validity of any model assumptions or resolving of any optical potential ambiguities with much less uncertainty. One such field which has recently received much attention, albeit without accompanying polarization data, is the study of refractive effects in terms of the normal, diffractive positive angle scattering from the near side of the target and the negative angle scattering from the far side. In this talk we present how positive and negative angle scattering and interferences thereof can be theoretically studied using polarization data firstly by adopting a trajectory picture, that is, in a semiclassical manner and secondly by taking the quantum mechanical approach of splitting the scattering process into its near and far-side contributions inasmuch as the Legendre functions, which occur in partial wave expansion within optical model, are rearranged accordingly.

A series of technical limitations is responsible for the fact that upto now a complete set of analysing power data is available only for some ${}^6\text{Li}$ (spin 1) and ${}^7\text{Li}$ (spin 3/2) elastic scattering from light (${}^{12}\text{C}$) and heavier (${}^{58}\text{Ni}$ say) targets at tandem energies. In view of this fact and due to the theoretical considerations introduced above, in this work we concentrate on developing a theoretical approach which is not only capable of simultaneously accounting for the observed cross section as well as analysing powers of all ranks, but also can incorporate a specific effect arising out of the size of the target.

To understand the target-size effect, we present the following argument for visualising elastic scattering of a light heavy-ion (HI) projectile like the lithium isotopes. Positive angle scattering is then the dominant process for scattering from a heavy target (say ${}^{58}\text{Ni}$ or heavier) since the negative angle contributions are heavily suppressed as projectiles which go around the target get more strongly absorbed. This is how we explain the relatively featureless Fresnel-type diffraction pattern for σ/σ_R of ${}^7\text{Li} + {}^{58}\text{Ni}$ elastic scattering at $E_{\text{lab}} = 20.3$ MeV [1] and the corresponding second rank tensor analysing power T_{20} is then well explained by taking recourse to the shape effect model [2]. This classical model associates changes in overlap between projectile and target at the point of closest approach to aligning quadrupole-deformed projectiles (here ${}^7\text{Li}$ with $Q\text{-moment} = -3.9 \text{ fm}^2$) with respect to various spin projections, since in a spin-polarized beam quadrupole moment and spin are co-axial. Thus the shape-effect model not only gives the correct (negative) sign of T_{20} for ${}^7\text{Li} + {}^{58}\text{Ni}$ beyond the grazing angle but also reproduces the magnitude for a reasonable choice of ${}^7\text{Li}$ quadrupole moment.

In contrast, for elastic scattering of lithium with the lighter target ${}^{12}\text{C}$ at comparable laboratory energies [3], the angular distribution of σ/σ_R shows wiggles for angles beyond the grazing angle and the simple shape effect model for obtaining the

analysing powers is automatically doomed to failure. Here, one can argue that the wiggles are due to interference effects between diffraction and negative angle scattering and therefore the simplified version of the shape effect model can be bidden good-bye. In this work we show how the 'nuclear matter overlap' ideology can be extended in a heavily modified form to negative angle scattering. Here we again re-iterate the notion that treating σ/σ_R and T_{20} on the same footing provides an extremely powerful methodology of obtaining a handle on negative angle scattering.

This report is divided into four sections. Polarization observables are briefly introduced and defined in sect. 2. Then we summarily discuss the semiclassical version of treating negative angle scattering in sect. 3 where the reader will be referred to our work on a general formalism of semiclassical theory of analysing powers. Next, in sect. 4 the quantum mechanical approach of separating the scattering process into positive and negative angle contributions is dealt with.

II - DEFINITION OF ANALYSING POWERS

Starting with the Schroedinger equation $H\psi = E\psi$, the scattering amplitude matrix M is defined by the asymptotic expansion of the total wave function Ψ as a sum of an incoming plane wave in a pure spin state m_0 and an outgoing spherical wave composed of all possible spin states. Thus

$$\psi \xrightarrow{r \rightarrow \infty} e^{i\vec{k}\vec{r}} |m_0\rangle + \frac{e^{iKr}}{r} \sum_m |m\rangle \langle m|M|m_0\rangle$$

where K is the wave number.

The centre-of-mass (c.m.) cross section $\frac{d\sigma}{d\Omega}(\theta_{c.m.}, \rho_{in})$ is obtained by transforming from the measured laboratory angle θ_{lab} to the corresponding c.m. angle. Thus,

$$\frac{d\sigma}{d\Omega}(\theta_{c.m.}, \rho_{in}) = \text{Tr} M^\dagger \rho_{in} M = \text{Tr} \rho_{in} M^\dagger M$$

where the spin state of the beam is described by the density matrix ρ_{in} in spin space.

Expanding $\rho_{in} = \sum_{0 \leq k \leq 2s} \tau_{kq} t_{kq}^* / (2s+1)$, where s is the projectile spin, k and q are the rank of the tensor and its projection and $\langle m' | \tau_{kq} | m \rangle = \sqrt{2k+1} c(sks; mqm')$ are the irreducible spherical matrices in spin space, one obtains

$$\frac{d\sigma}{d\Omega}(\theta_{c.m.}, \rho_{in}) = \frac{1}{2s+1} \sum_{kq} t_{kq}^* \text{Tr}_{kq} M^\dagger M = \frac{\text{Tr} M^\dagger M}{2s+1} \{1 + \sum_{k>1} t_{kq}^* \tau_{kq}\}.$$

Here, $\frac{\text{Tr} M^\dagger M}{2s+1} \equiv \left(\frac{d\sigma}{d\Omega}\right)_{unpol.}$

The t_{kq} 's denote the 'prepared' beam polarization and the T_{kq} 's are the measured analysing powers.

Specialisation

Rank 1 ($k = 1$): For the rank 1 case the beam is 'prepared' in a way such that the matrix ρ has the following elements:

$$\langle m' | \rho_{in} | m \rangle = \delta_{mm'} \frac{1+m/s}{2s+1},$$

that is, the occupation number is a linear function of the magnetic substates. Clearly then, $\rho_{in} = \frac{1}{2s+1} (1 + \frac{1}{s} \vec{s} \cdot \vec{e})$ and in this construction the only non-zero t_{1q} is t_{10} .

Such a beam is called a 'vector polarized' beam. If now one measures the transverse vector (or first rank) analysing power, called T_{10} , by taking the quantisation axis such that $\hat{e} || \vec{p}_i \times \vec{p}_f$, then this 'transverse' quantity is

$$T_{10} = \frac{1}{t_{10}} \frac{(\frac{d\sigma}{d\Omega})_{\text{pol.}} - (\frac{d\sigma}{d\Omega})_{\text{unpol.}}}{(\frac{d\sigma}{d\Omega})_{\text{unpol.}}}.$$

For the transversity frame the choice of axis is $\vec{p}_i \times \vec{p}_f || \hat{e}_z$ and for the Madison frame [4] one chooses $\vec{p}_i \times \vec{p}_f || \hat{e}_y$. For rank 1 the 'transverse' T_{10} is simply proportional to 'Madison' iT_{11} (as a whole a real quantity!), i.e., $T_{10} \propto iM_{11}$. Further details on this subject and interrelations among the various conventions of defining polarization observables can be obtained from ref. [4].

Rank 2 ($k = 1$): Here we shall simplify the discussion by directly considering the situation for spin 3/2. In this case the beam is 'prepared' such that only $t_{20} = 1$ and all other t_{kq} 's are zero. This is achieved, say, by having a quadratic (parabolic) behaviour of the occupation number as a function of the magnetic projection as follows:

$$\langle m' | \rho_{in} | m \rangle = \begin{cases} \frac{1}{2} & \text{for } m' = m = 3/2 \\ 0 & \text{otherwise} \end{cases}$$

Such a beam is called 'aligned' and the transverse tensor (or second rank) analysing power is

$$T_{20} = \frac{(\frac{d\sigma}{d\Omega})_{\text{aligned}} - (\frac{d\sigma}{d\Omega})_{\text{unpol.}}}{(\frac{d\sigma}{d\Omega})_{\text{unpol.}}}.$$

III - SEMICLASSICAL TREATMENT OF POSITIVE AND NEGATIVE ANGLE SCATTERING

In the following we only shall briefly indicate those steps in the formalism of treating negative angle scattering essential for our calculations. Detailed treatment of positive angle scattering and polarization observables within the semiclassical framework is given in our paper, vide ref. [5].

We start with taking the real central potential v_c to be the dominant interaction and treat v_c in a classical approximation to obtain trajectories of the projectile. All the rest of the potentials, be they absorptive central (w_c) or complex spin-orbit (U) are treated perturbatively. The absorption, governed by w_c , therefore, takes place simply while the projectile moves on its trajectory and the spin-dependent interactions, caused by U , generate a time-evolution of the projectile spin state again without affecting the trajectories. As a sequel to these assumptions the S-matrix factorizes into a product of two terms, the first factor being the S-matrix for central potentials and the other being a matrix B in spin space, which narrates the effects of spin-dependent interactions on the spin state of the projectile. Next, the S-matrix so obtained is inserted into a semiclassical expression [6] for the matrix M of scattering amplitudes. The usual partial wave sum for the scattering amplitude is transformed into an integration over trajectories and the M-matrix is evaluated by the method of stationary phases [7]. Finally, from the M-matrix the analysing power for elastic polarized HI scattering are calculated applying standard definitions [4] used for describing polarization phenomena.

Starting with the full time-dependent Schroedinger equation for the relative motion of particles with a real central interaction, we make the following simplifications as regards the trajectories. Firstly, the wave packet is a narrow one and secondly, its centre moves along the trajectory. The Morse saddle point equations for absolute values of L are

$$\frac{\partial}{\partial L} 2\delta_c(L) + \epsilon\theta + 2\pi\nu = 0 \quad (\epsilon = \pm 1) \quad (1)$$

and the general behaviour of the classical deflexion function

$$\theta_c(L) = \partial 2\delta_c(L) / \partial L$$

is sketched in fig. 1 of ref. [5], where it can be seen that θ_c is determined essentially by Coulomb repulsion for large L values and it goes through the rainbow angle θ_R at $L = L_R$ and becomes infinite for grazing angular momentum L_g . In table 1 of ref. [5] the rainbow parameters are presented for the currently available data sets for the two projectiles ${}^6\text{Li}$ and ${}^7\text{Li}$.

For the sake of methodological consistency within the semiclassical framework, δ_c , the real central phase shift is taken to be the WKB one corresponding to the real central potential v_c and the central absorptive coefficient, α_c , is defined by

$$\alpha_c(L) = -\frac{1}{\hbar} \int_{-\infty}^{\infty} w_c(R_t) dt .$$

Two graphical solutions of eq. (1) for a specific $\theta > \theta_R$ are also depicted in fig. 1 of ref. [5]. If we have $\theta < \theta_R$, there exist also two solutions of eq. (1) for $v = 0$, $\varepsilon = -1$, i.e., for positive deflexion angles θ . These last two solutions become complex when varying θ from values below θ_R to those above of it. As in ref. [8], approximate complex solutions are calculated by expanding θ_c around L_R and solving

$$\theta_R + \frac{1}{2} (L - L_R)^2 \theta_R'' - \theta = 0 ,$$

θ_R'' being the second derivative of θ_c at $L = L_R$. Thus, for $\theta < \theta_R$, L_0 which represents actually two values of angular momenta, one on the ascending and the other on the descending side of the deflexion function, corresponds to a pair of positive angle contributions denoted by g_0 . Also for $\theta < \theta_R$, L_1 lying as it does between 0 and $-\pi$ generates the negative angle contribution g_1 and L_2 lying between $-\pi$ and -2π gives the negative angle contribution for a single orbiting around the target called g_2 etc. For $\theta > \theta_R$ one of the pair of complex solutions L_0 must be taken into consideration aside from the real solutions of eq. (1), i.e., L_1, L_2 etc. The other complex solution is to be discarded because this would have an exponentially increasing contribution to the scattering amplitude. In other words, for a Fresnel diffraction pattern of the cross section, the diffraction amplitude g_0 dominates and if one has a wiggly σ/σ_R , this is caused by interference between g_0 and g_1 .

The next step consists of introducing spin-dependent potentials into the above-discussed procedure for central potentials and writing down the time-dependent Schrödinger equation for the spin-state evolution matrix B . This generates spin-orbit phase shifts δ_{so} given by

$$2\delta_{so}(L) = -\frac{L}{\hbar} \int_{-\infty}^{\infty} v_{so}(R_t) dt .$$

The physical meaning of this result is that projectiles in particular eigenstate of $\vec{s} \cdot \vec{L}$ will stay in the same one while moving along a trajectory. The real spin-orbit phase shift $2m\delta_{so}$ and the spin-orbit absorption coefficient α_{so} , for $w_{so} \neq 0$, depend on m , the eigenvalue of $\vec{s} \cdot \vec{L}$. Needless to say that the introduction of spin-dependent potentials modifies the saddle point equation (1) accordingly, encompassing spin-dependent forces and spin-flip processes. As a result of the factorization property mentioned above, we now have, associated with each g_i , a corresponding multiplicative factor h_i due to the spin-dependent potentials.

When diffraction scattering dominates, say, for a heavy target, i.e., σ/σ_R shows Fresnel pattern, we know from above that then only g_0 contributes to f_c . Calculations were done for iT_{11} for such a situation and the result is shown in fig. 4 of ref. [5]. The agreement with data is excellent inasmuch as the calculation is parameter-free.

We now present the theory for calculating g_1 , i.e., consider a scattering process like ${}^6\text{Li} + {}^{12}\text{C}$ where the diffraction term plus non-orbiting negative angle term and interferences thereof all play a role due to the smaller target size. The input potentials [3] obtained by optical model fit are the real and the imaginary central potentials and the real and the imaginary spin-orbit potentials.

The procedure is divided into three steps.

- As for the positive angle case, one determines the deflexion function θ and obtains therefrom the rainbow parameters θ_R , L_R and θ_R'' , where the double dash indicates the second derivative with respect to L and the corresponding rainbow absorption coefficients $\alpha_c(L_R)$ and $\alpha_{so}(L_R)$ and the rainbow spin-orbit phase shift $2\delta_{so}(L_R)$ and its derivative $2\delta_{so}'$.
- Then one determines the range R of R_0 values, R_0 being the distance of closest approach, for which $-\pi \leq \theta \leq 0$, i.e., one is in the negative angle range.
- Divide the range R into parts so that oscillations in the experimental data can be reproduced. Note that the relationship between R_0 and $\theta_{c.m.}$ is not linear. Concretely speaking, if experimental data exist between, say, 30° and 130° , i.e., within an angular range of 100° and oscillations need to be reproduced to within 0.5° , one then divides R into approximately 200 parts, taking care of slight non-linearity. Then, for each of these values of R_0 , one calculates L and θ and the absorption coefficients α_c and α_{so} along with $2\delta_{so}$. In addition, the following integral is needed, namely,

$$\chi = - \int_L^{L_R} \theta(L') dL'$$

and the derivatives θ' , α_c' , $2\delta_{so}'$, θ'' and $2\delta_{so}''$ with respect to L .

After having numerically obtained these many quantities, we can now write down the last set of formulae to obtain σ/σ_R and iT_{11} . Thus, the diffraction and the non-orbiting negative angle amplitudes are, respectively,

$$|g_0| = \sqrt{2\pi L_R} \left[\frac{2}{|\theta_R''|} \right]^{1/3} |Ai(x)| e^{-\alpha_c(L_R)} \quad \text{with} \quad x = \left[\frac{2}{|\theta_R''|} \right]^{1/3} (|\theta| - \theta_R)$$

and $|g_1| = \sqrt{\frac{L}{\theta'}} e^{-\alpha_c}$, Ai being the Airy function, and the phase

$$\psi = \chi + (L + L_R)|\theta| - \frac{\pi}{4} + \frac{\pi}{2} (1 - \text{Sign Ai}(x)).$$

The corresponding spin-dependent functions, h_i , are

$$h_0 = -2\delta_{so}'(L_R) \left[\frac{2}{|\theta_R''|} \right]^{1/3} \cdot \frac{Ai'(x)}{Ai(x)}$$

$$h_1 = -\frac{2\delta_{so}'}{2L\theta'} + \frac{\theta''2\delta_{so}'}{2(\theta')^2} - \frac{2\delta_{so}''}{2\theta'} + \frac{\alpha_c 2\delta_{so}'}{\theta'}$$

Thus, the unpolarized cross section is

$$\frac{\sigma}{\sigma_R}(\theta) = \frac{8E(\hbar c)^2}{m_{red}(z_1 z_2 e^2)^2} \cdot \frac{\sin^4(\frac{\theta}{2})}{\sin|\theta|} F_0$$

and the first rank vector analysing power is

$$iT_{11}(\theta) = \frac{F_1}{F_0} 2\sqrt{\frac{s(s+1)}{6}}$$

$$\text{with } F_0 = |g_0|^2 + |g_1|^2 + 2|g_0| |g_1| \cos \psi$$

$$\text{and } F_1 = -\{|g_0|^2 + |g_0| |g_1| \cos \psi\} \{h_0 - \alpha_{so}(L_R)\}$$

$$+ \{|g_1|^2 + |g_0| |g_1| \cos \psi\} \{h_1 - \alpha_{so}\}$$

$$- |g_0| |g_1| \sin \psi \{2\delta_{so} + 2\delta_{so}(L_R)\}$$

For each of the numerous R_0 values, one thus has to calculate several integrals and differential coefficients along the trajectory. In this process, extreme care has to be given to avoid convergence problems, particularly for integrals near R_0 . Computational work is in progress and the typical time for one full calculation is about 10 CPU minutes on a CRAY computer. This clearly demonstrates that one has reached the limit of viability of such semiclassical calculations numerically and therefore in the next section we shall present how to go about tackling this problem by a method which should be more suited for it, namely the quantum mechanical procedure.

IV - QUANTUM APPROACH TO POSITIVE AND NEGATIVE ANGLE SCATTERING

In order to simplify the discussion, we consider for the time being only central potentials. Starting from the partial wave sum for the scattering amplitude

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} P_l(\cos \theta) (s_l - 1)(2l + 1) ,$$

we decompose the Legendre polynomials as follows

$$P_l = \frac{1}{2} (P_l + i \frac{2}{\pi} Q_l) + \frac{1}{2} (P_l - i \frac{2}{\pi} Q_l)$$

where Q_l are the Legendre functions of the second kind [9].

$$\text{Put } Q_l^{(-)} = \frac{1}{2} (P_l + i \frac{2}{\pi} Q_l)$$

$$Q_l^{(+)} = \frac{1}{2} (P_l - i \frac{2}{\pi} Q_l) .$$

$$\text{Then, } f(\theta) = f^{(-)} + f^{(+)}$$

$$\text{with } f^{(\pm)} = \frac{1}{2ik} \sum_{l=0}^{\infty} Q_l^{(\pm)} (s_l - 1)(2l + 1)$$

and

$$\frac{\sigma}{\sigma_R} \equiv |f|^2 = |f^{(-)}|^2 + |f^{(+)}|^2 + \text{interference terms.}$$

Semiclassically, the amplitude $f^{(-)}$ corresponds to the diffractive/positive angle contribution and $f^{(+)}$ to the refractive/negative angle contribution.

Satchler and coworkers [10] have coined the phrase 'near-side' and 'far-side' for the two cases respectively. This association is obvious, since

$$Q_l^{(\pm)} \approx \frac{e^{i\{\pm i(1 + \frac{1}{2})\theta - i\frac{\pi}{4}\}}}{\sqrt{2\pi(1 + \frac{1}{2}) \sin \theta}} \quad \text{for large } l.$$

The extension to include spin-dependent potentials is relatively straightforward, albeit cumbersome. For example, we now need the associated Legendre functions of the second kind instead of the ordinary ones since magnetic projection is of paramount importance now. In particular, we note that in the case of $\text{Li} + \text{Ni}$ at $E_{\text{lab}} \leq 20$ MeV scattering is essentially near-side. Contrarily, in the case of $\text{Li} + \text{C}$ both near-side and far-side amplitudes contribute and interfere. Clearly, the ${}^7\text{Li}-\text{T}_{2q}$ near-side can be expected to behave as the shape effect model predicts, while the far-side T_{2q} 's do not. Work is in progress to introduce these changes into the spin 3/2 optical model code LINA.

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