A general numerical solution of dispersion relations for the nuclear optical model

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A general numerical solution of the dispersion integral relation between the real and the imaginary parts of the nuclear optical potential is presented. Fast convergence is achieved by means of the Gauss-Legendre integration method, which offers accuracy, easiness of implementation and generality for dispersive optical model calculations. The use of this numerical integration method in the optical-model parameter search codes allows for a fast and accurate dispersive analysis.

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For many years the evaluation of reaction cross section and elastic scattering data has relied on the use of the optical model. A significant contribution during the last two decades can be considered the work of Mahaux and co-workers on dispersive optical-model analysis [1–3]. The unified description of nuclear mean field in dispersive optical-model is accomplished by using a dispersion relation (DR), which links the real and absorptive terms of the optical model potential (OMP). The dispersive optical model provides a natural extension of the optical model derived data into the bound state region. In this way a physically self-consistent description of the energy dependence of the OMP is obtained and the prediction of single-particle, bound state quantities using the same potential at negative energies became possible. Moreover additional constraint imposed by DR helps to reduce the ambiguities in deriving phenomenological OMP parameters from the experimental data. The dispersive term of the potential $\triangle V(E)$ can be written in a form which is stable under numerical treatment [4], namely:

$$\triangle V(E) = \frac{2}{\pi}(E - E_F)\int_{E_F}^{\infty} \frac{W(E') - W(E)}{(E' - E_F)^2 - (E - E_F)^2} dE' \tag{1}$$

where E is the incident projectile energy and E_F is the Fermi energy for the target system.

The imaginary OMP can be written as the sum of volume and surface contributions: $W(E) = W_V(E) + W_S(E)$. It is useful to represent the variation of surface $W_S(E)$ and volume absorption potential $W_V(E)$ depth with energy in functional forms suitable for the DR optical model analysis. An energy dependence for the imaginary volume term has been suggested in studies of nuclear matter theory:

$$W_V(E) = \frac{A_V(E - E_F)^n}{(E - E_F)^n + (B_V)^n} \tag{2}$$

where A_V and B_V are undetermined constants. Mahaux and Sartor [3] have suggested $n = 4$, while Brown and Rho [**?**], $n = 2$. An energy dependence for the imaginary-surface term has been suggested by Delaroche *et al* [4] to be:

$$W_S(E) = \frac{A_S(E - E_F)^m}{(E - E_F)^m + (B_S)^m} \exp(-C_S|E - E_F|) \tag{3}$$

where $m = 4$ and A_S, B_S and C_S are undetermined constants. Other energy functionals are suggested in the literature [2,5]. According to equations (2) and (3) the imaginary part of the OMP is assumed to be zero at $E = E_F$ and nonzero everywhere else. A more realistic parametrization of $W_V(E)$ and $W_S(E)$ forces these terms to be zero in some region around the Fermi energy. A physically reasonable energy for defining such a region is the average energy of the single-particle states E_P [1]. We can define the offset-energy E_{of} for both the particle and the hole region by the relation:

$$E_{of} = E_P - E_F \tag{4}$$

Therefore a new definition for imaginary part of the OMP can be written as:

$$W_V(E) = 0, \text{ for } E_F < E < E_p \tag{5}$$

$$W_V(E) = \frac{A_V(E - E_P)^n}{(E - E_P)^n + (B_V)^n}, \text{ for } E_P < E \tag{6}$$

and likewise for surface absorption. The symmetry condition $W(2E_F - E) = W(E)$ is used to define imaginary part of the OMP for energies below the Fermi energy. We assume below that equations (2) and (3) are modified according to (5) and (6).

In a recent work [6], analytical solutions of the dispersion integral relation between the real and imaginary parts of the nuclear optical model were proposed. The main reason for such effort was the slow convergence of the Simpson integration method (SIM) for solving the DR integral (1). The authors needed 6000 steps in total (50 keV each) to calculate (1) up to 300 MeV. Beyond 300 MeV, the integral was approximated by assuming that the numerator of its integrand become constant-valued [6]. Obviously this lengthen very much the OMP calculations, so they derived approximate analytical solutions of the integral (1) for usual forms of the imaginary OMP, including those given by (2) and (3). However the approximate analytical solution recently derived [6] depends, of course, on assumed functional form of the imaginary part of the OMP.

In this work we propose a fast and general numerical solution for calculation of the DR integral (1), based on Gauss-Legendre integration method (GLIM) [7]. Integral in a finite interval (a, b) can be converted by linear transformation to the integral in the interval $(-1, 1)$ and then approximatted according to the following formula:

$$\int_{-1}^{1} f(x)dx = \sum_{i=1}^{N} W_i^N f(X_i^N) \tag{7}$$

where W_i^N and X_i^N are weights and abscissas corresponding to the N point Gauss-Legendre integration method [7]. In this work we were using N=10 for each interval. At the first look of equation (1) we could be tempted to use Gauss-Laguerre integration method [7]. However beyond some energy cut-off E_{cut}, such that $E_{cut} >> E$, the integral can be very well approximated by assuming that the numerator of its integrand becomes constant-valued. In this case we obtain the following relation:

$$\triangle V_{res}(E) = \frac{2}{\pi}(E - E_F)\int_{E_{CUT}}^{\infty} \frac{W(E') - W(E)}{(E' - E_F)^2 - (E - E_F)^2}dE' = \frac{W(E)}{\pi}\log\left(\frac{E_{cut} - (E - E_F)}{E_{cut} + (E - E_F)}\right) \tag{8}$$

Therefore we can apply GLIM from E_F up to E_{cut} for a finite interval. This option was shown to be more accurate for a given problem. This method is suitable for practically any type of DR integrand function. Moreover the implementation of this method in optical model parameter search code is straightforward. The method is compared with SIM and, for the surface dispersive contribution, with the results of analytical integration [6]. The parameters of the dispersive OMP used in our tests correspond to the "partially constrained set" derived in Ref. [8] to describe neutron scattering on ^{209}Bi up to 80 MeV incident energy (see Table II, [8]). For ^{209}Bi the Fermi energy is equal to -5.98 MeV and the offset energy was taken as 3.26 MeV, assuming the average energy of the particle states is the same of ^{208}Pb [8].

In order to attain a good accuracy in the numerical integration (1), attention must be paid to the behavior of the integrand,

$$I_{E,E_F}(E') = \frac{W(E') - W(E)}{(E' - E_F)^2 - (E - E_F)^2} \tag{9}$$

The integrand $I_{E,E_F}(E')$ for dispersive surface correction ($W_S(E)$ given by equation (3)) is shown in Figure 1. As a result of the exponential damping in the surface OMP the integrand $I_{E,E_F}(E')$ decreases sharply above 5-6 MeV. This behavior suggests that separation of the integration interval is desirable in order to improve the accuracy of the numerical integration method. It should be stressed that exponential damping contained in functional form (3) reflects the physical fact that surface absorption is expected to decrease fast as the incident energy is increased. This behavior is observed in almost any phenomenological OMP analysis, so dividing integration interval is not a recipe for functional form (3), but should be valid practically for any imaginary surface absorption energy functional. We decided to divide the interval in two parts from E_F up to $E_{int} = 10MeV$ and then from E_{int} up to some cut-off energy in the integral. The E_{int} position was chosen in order to guarantee monotonous behavior of the integrand in the interval from E_{int} up to infinity. Practically it is enough to select E_{int} slightly larger than the energy of the maximum value of the integrand. The cut-off energy E_{cut} in the DR integral for dispersive surface correction was taken at 1000 MeV. Beyond 1000 MeV we used equation (8) to estimate contribution from the tail of the integral. This residual value was added to both numerical methods. The dispersive surface correction $\triangle V_S(E)$ calculated by GLIM (using 20 integration points) and SIM (100 keV step, more than 10000 integration points) were compared with analytical solution from Ref. [6]. Maximum deviation between any of the three methods was less than 1 KeV in the whole energy range from E_F up to 150 MeV energy.

A similar behavior of the integrand $I_{E,E_F}(E')$ is observed for the case of the dispersive volume correction ($W_V(E)$ given by equation (2)). However the integrand $I_{E,E_F}(E')$ is smoother and has longer tail than was the case for

surface correction. The reason is that no exponential damping is introduced here. Similarly to what we did before, we divided the interval in two parts from E_F up to $E_{int} = 40MeV$ and then from E_{int} up to cut-off energy E_{cut}. Beyond 1000 MeV we used equation (8) to estimate contribution from the tail of the integral. The integration was performed by GLIM and SIM. An excellent agreement is achieved between both numerical methods.

In conclusion, we have proposed an accurate and general numerical method for calculating dispersive contribution to the real part of the optical model potential. The method is very fast and thanks to its computational simplicity should be easy to implement in current generation of the optical model parameter search codes. We stress that, unlike analytical solution, any energy functional representation of the imaginary part of the OMP can be treated in our approach. These properties make the method very useful for introduction of the dispersive optical model relation in large scale nuclear data calculations.

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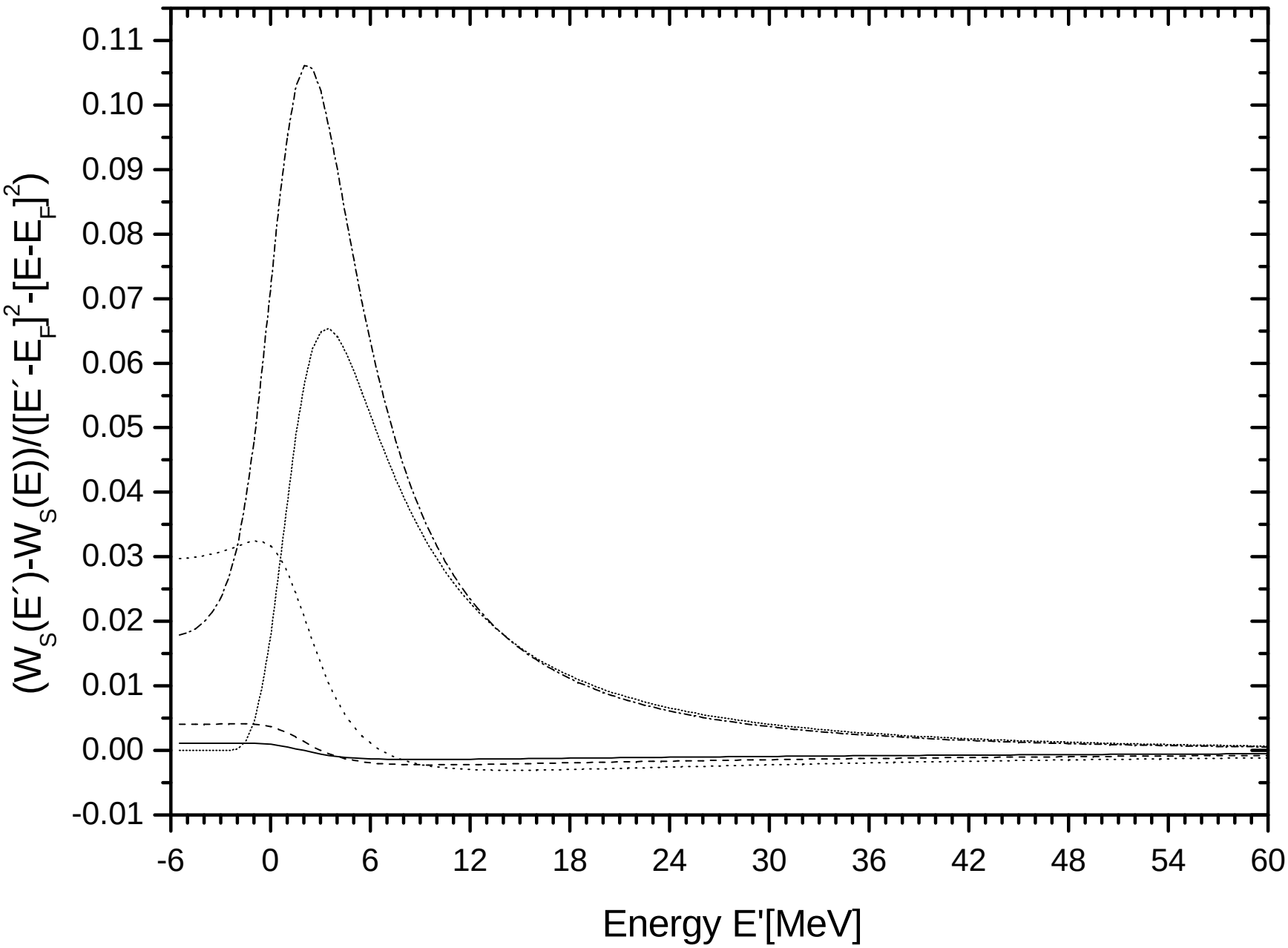
FIG. 1. Energy dependence of the DR integrand $I_{E,E_F}(E')$ for the dispersive surface contribution of the imaginary OMP (short dottted line) $E = E_F + 0.25MeV$, (dash dotted line) $E = 0$, (dotted line) $E = 10MeV$
(dashed line) $E = 30MeV$, (solid line) $E = 50MeV$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-6
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12
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24
30
36
42
48
54
60
Energy E'[MeV]
(W_S(E´)-W_S(E))/([E´-E_F]^2-[E-E_F]^2)