Calculation of the Shell-Model Potential from the Optical-Model Potential

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A dispersion-relation approach is developed for deriving the shell-model potential from the optical-model potential, i.e., for extrapolating the mean field from positive towards negative nucleon energies. This method is applied to neutrons in ^{208}Pb. The average neutron-nucleus potential is assumed to have a Woods-Saxon shape; its depth, radius, and diffuseness are calculated for nucleon energies with range from −20 to +40 MeV.

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The nuclear mean field $M(r;E)=V(r;E)+iW(r;E)$ plays a central unifying role in the interpretation of many nuclear structure and reaction properties; r denotes the distance from the nuclear center and E the nucleon energy. For $E>0$, M is called the optical-model potential and is used for the description of scattering cross sections. For $E<0$, $V(r;E)$ is called the shell-model potential and describes the single-particle states observed in nucleon transfer reactions. Although the mean field is a continuous function of the energy, its behavior as the energy changes sign is not simple[1] because of the coupling between the single-particle degree of freedom (the elastic channel in the terminology used in reaction theory) and other degrees of freedom (associated with core excited states in the terminology used in nuclear-structure theory or with inelastic channels in the terminology used in reaction theory). Besides giving rise to an intricate energy dependence of $V(r;E)$, this coupling is responsible for the existence of an imaginary part in the mean field. It is therefore natural that these two features are interrelated. In the present paper, we use the empirical information on $W(r;E)$ to obtain detailed information on the behavior of $V(r;E)$ as E changes sign.

We make the standard assumption that $V(r;E)$ has a Woods-Saxon shape:

$$V(r;E)=\frac{-U_V}{1+\exp[(r-R_V)/a_V]}. \tag{1}$$

The main purpose of the present Letter is to propose a method for the extrapolation of the potential parameters U_V, R_V, and a_V from positive to negative energies. This method will be applied to the n-^{208}Pb system. This extrapolation is of great interest since much more information on these parameters is available at positive than at negative energies. Indeed, in a scattering experiment many experimental data (differential and polarization cross sections at many angles) are available for a chosen bombarding energy. In contrast, the empirical information on $V(r;E)$ for $E<0$ is available only at the discrete single-particle (SP) energies E_j associated with bound SP excitations; furthermore, this information is usually limited to the SP energies E_j themselves, i.e., to one datum point at a few discrete energies.

The microscopic nucleon-nucleus potential can be identified with the mass operator $\mathcal{M}(\mathbf{r},\mathbf{r}';E)$[1] which as indicated is a nonlocal, energy-dependent operator. We write this mass operator in the schematic form $\mathcal{M}=\mathcal{V}+i\mathcal{W}$. It is analytic in the upper half of the complex E plane, and therefore satisfies the following dispersion relation (DR)[1]:

$$\mathcal{V}(\mathbf{r},\mathbf{r}';E)=\mathcal{V}_{\rm HF}(\mathbf{r},\mathbf{r}')+\frac{\rm P}{\pi}\int_{-\infty}^{\infty}\frac{\mathcal{W}(\mathbf{r},\mathbf{r}';E')}{E'-E}\,dE' \tag{2}$$

$$=\mathcal{V}_{\rm HF}+\Delta\mathcal{V}(E), \tag{3}$$

say, where P denotes principal value. This DR can be viewed as a consequence of causality[2] and is the analog of the Kramers-Kronig relation in optics. The contribution $\Delta\mathcal{V}(E)$ depends upon E: It is the "dynamic part"[1,3] of the mass operator; by analogy with optics, we call it the dispersive contribution to the mean field. It is due to the coupling between the elastic and nonelastic channels. It vanishes when $\mathcal{W}$ vanishes, i.e., when nucleon-nucleon collisions are omitted. Then, $\mathcal{V}$ reduces to $\mathcal{V}_{\rm HF}$ which is thus the potential which is obtained when nucleon-nucleon correlations are omitted in the target, and when the latter is assumed to remain in its ground state throughout the collision process. The quantity $\mathcal{V}_{\rm HF}$ will therefore be called the Hartree-Fock (HF) component of the mean field[1,4]; it is real, nonlocal, and independent of energy.

One can construct local potentials which are equivalent to nonlocal ones, in the sense that they yield the same scattering phase shifts and SP energies. These local equivalent potentials depend smoothly upon energy. It can be argued[1,5] plausibly that the DR is also obeyed approximately by these local equivalent potentials. It then reads

$$V(r;E)=V_{\rm HF}(r;E)+\frac{\rm P}{\pi}\int_{-\infty}^{\infty}\frac{W(r;E')}{E'-E}\,dE', \tag{4}$$

where for instance $V_{\rm HF}(r;E)$ is the local equivalent of $\mathcal{V}_{\rm HF}(\mathbf{r},\mathbf{r}')$. We assume that $W(r;E')$ is symmetric about $E'=E_{\rm F}$,[1,5] where $E_{\rm F}$ is the Fermi energy which lies half-

way between the two valence shells ($E_F = -5.65$ MeV for neutrons in ^{208}Pb). Then $V(r;E_F) = V_{HF}(r;E_F)$: At the Fermi energy, the shell-model potential becomes identical to its Hartree-Fock component.

It is difficult to make direct use of Eq. (4), because the radial dependence of the imaginary part $W(r;E')$ is not very accurately known empirically. However, compilations of empirical optical-model potentials show[6] that the energy dependence of the radial moments $[r^q]_V$ and $[r^q]_W$, where, e.g.,

$$[r^q]_W(E) = \frac{4\pi}{A}\int_0^\infty W(r;E) r^q dr \quad (5)$$

is quite well determined empirically, for exponents q which range from 0.4 to 4. This property is useful because the radial moments satisfy the following DR:

$$[r^q]_V(E) = [r^q]_{HF}(E) + \frac{P}{\pi}\int_{-\infty}^{\infty} \frac{[r^q]_W(E')}{E'-E} dE', \quad (6)$$

which immediately derives from Eq. (4). We shall use the DR (6) to evaluate $[r^q]_V(E)$ for three different values of the exponent q, namely 0.8, 2, and 4. From these three radial moments we shall then determine the three Woods-Saxon parameters U_V, R_V, and a_V. Note that $[r^2]_V$ is the familiar volume integral per nucleon and the ratio $[r^4]_V/[r^2]_V$ is the mean-square radius of the real part of the potential.

The energy dependence of the quantity $[r^q]_{HF}(E)$ is due to the replacement of the nonlocal HF potential by its local equivalent; $[r^q]_{HF}(E)$ is therefore a smooth function of E, which can be approximated by a linear law: $[r^q]_{HF}(E) = B_q + C_q E$, where B_q and C_q are adjustable parameters. Equation (5) then gives $[r^q]_V(E)$ as a sum of the linear function of energy $[r^q]_{HF}(E)$ and of the dispersive contribution $[r^q]_{\Delta V}(E)$. The latter has a typical energy dependence when E approaches E_F because $[r^q]_W(E)$ then rapidly varies with energy due to the closure of nonelastic channels. This property is illustrated in Fig. 1(a) in the case of the volume integral per nucleon $[r^2]_W(E)$; the full curve represents a least-squares fit with the following Brown-Rho (BR) expression[7]:

$$[r^q]_W(E) = -w_q \frac{(E-E_F)^2}{(E-E_F)^2+\sigma_q^2}, \quad (7)$$

in the case $q=2$. Here, w_q and σ_q are two adjustable parameters. We have also performed similar fits for $q=0.8$ and 4. The parametrization (7) enables one to calculate algebraically, for all values of E, the quantity $[r^q]_{\Delta V}(E)$, i.e., the second term on the right-hand side of Eq. (6).[7]

Then the remaining unknowns for the evaluation of $[r^q]_V(E)$ are the two parameters B_q and C_q which appear in $[r^q]_{HF}(E)$. Since we want to extrapolate the mean field from positive to negative energies, we determine B_q and C_q by a least-squares fit to the empirical values[8] of $[r^q]_V(E)$ for $E>0$. This yields $[r^q]_V(E)$ as algebraic functions of E for all energies. For instance, the calculated value of $[r^2]_V(E)$ is represented by the

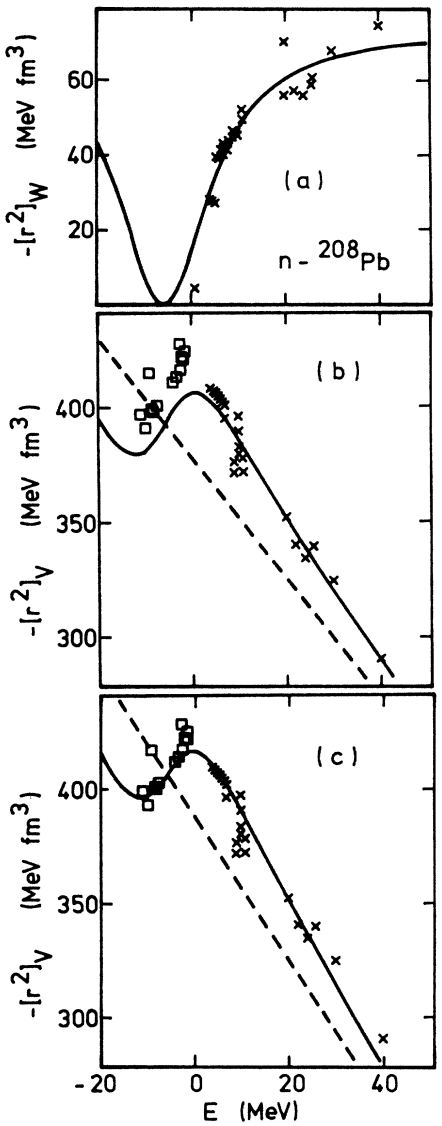

FIG. 1. Energy dependence of the volume integrals per nucleon of the imaginary and real parts of the mean field for neutrons in ^{208}Pb. The crosses are empirical values (Ref. 8) associated with phenomenological optical-model potentials. The curve in (a) is a least-squares fit of the empirical $[r^2]_W$ with the BR parametrization, Eq. (7). The lines in (b) represent the calculated values of $[r^2]_{HF} = B_2 + C_2 E$ (dashed line) and of $[r^2]_V$ (solid line), as obtained by our determining B_2 and C_2 from a least-squares fit to the empirical values represented by the crosses; the open squares are located at the experimental SP energies E_j and represent values of $[r^2]_V(E_j)$ obtained by our adjusting the Woods-Saxon depth $U_V(E_j)$ while using the calculated shape parameters $R_V(E_j)$, $a_V(E_j)$ being associated with the extrapolated values of $[r^q]_V(E_j)$ ($q=0.8$, 2, 4). The curves in (c) have the same meaning, except that the squares are now included in the data set used in the least-squares determination of B_q and C_q.

solid curve in Fig. 1(b).

Once the three moments $[r^q]_V(e)$ ($q=0.8$, 2, 4) are known, one can calculate the dependence upon E of the three parameters U_V, R_V, a_V of the Woods-Saxon mean field $V(r;E)$. The dependence upon E of $r_V=R_VA^{-1/3}$ ($A=208$) and of the diffuseness a_V is represented by full curves in Fig. 2.

The reliability of our procedure can be evaluated from the following consistency check which, at the same time, provides a method for the improvement of the extrapolation towards negative energies. We introduce a typical spin-orbit potential from Dudek, Szymanski, and Werner.[9] Using the calculated values of $R_V(E_j)$ and $a_V(E_j)$ at an experimental SP energy E_j, we determine the depth $U_V(E_j)$ which reproduces this experimental E_j. These three parameters $R_V(E_j)$, $a_V(E_j)$, and $U_V(E_j)$ determine the radial moments $[r^q]_V(E_j)$. These are represented by the open squares in Fig. 1(b), in the example $q=2$. These open squares should fall on the solid curve if our extrapolation were exact. Figure 1(b) shows that the trend of the energy dependence is correct but that a small deviation exists; the same feature holds for $q=0.8$ and $q=4$.

We thus included the values associated with these open squares in the data set used for the least-squares determination of the parameters B_q and C_q, and iterated until the calculated curve $[r^q]_V(E)$ is stable. It turns out that this only slightly modifies the calculated parameters $r_V(E)$ and $a_V(E)$, while the depth U_V is increased by about 2%. The final values of $U_V(E)$, $r_V(E)$, and $a_V(E)$ are given by the full curves in Fig. 2. Between 5 and 20 MeV, the depth U_V weakly depends upon energy, while r_V rapidly decreases. These features are in good agreement with recent experimental findings.[10] The energy dependence of r_V near E_F reflects the importance of the coupling between the SP states and the vibrations of the nuclear surface.[1] The calculated values of a_V are less reliable because they are sensitive to small changes of the radial moments $[r^q]_V$; however, the calculated values of $U_V(E)$ and $r_V(E)$ are hardly modified if one assumes that a_V is independent of energy, so that our calculated values of $U_V(E)$ and $r_V(E)$ are quite reliable.[11]

The final values of $[r^2]_V(E)$ are represented by the solid curve in Fig. 1(c). Their agreement with the empirical values of $[r^2]_V$ is quite good for E positive as well as negative. An agreement of similar quality is obtained for the moments associated with $q=0.8$ and $q=4$. Figure 1(c) confirms that the energy dependence of $V(r;E)$ is not simple when E changes sign. Note that for E somewhat smaller than E_F the mean field is less attractive than in the HF approximation, while the opposite is true for E somewhat larger than E_F. This explains why HF calculations yield too a large value for the energy gap between particle and hole SP states.[12]

In phenomenological analyses, the shell-model potential is assumed to have the Woods-Saxon shape (1), with

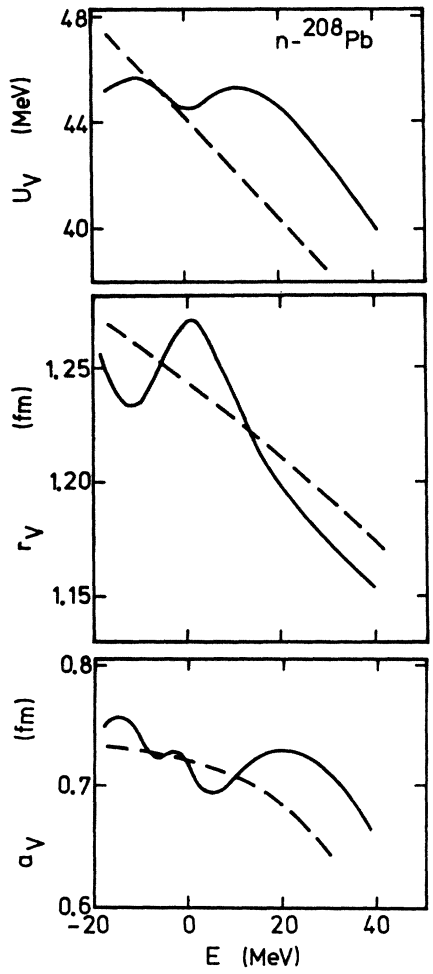

FIG. 2. Energy dependence of the parameters (U_V,r_V,a_V) of the Woods-Saxon mean field, Eq. (1). The dashed lines are derived from the moments $[r^q]_{HF}(E)$ of the HF contribution, $q=0.8$, 2, and 4; the solid curves are obtained from the moments $[r^q]_V(E)$ of the real part of the full potential.

energy-independent geometrical parameters R_V and a_V. Figure 2 shows that this parametrization is quite crude in the vicinity of the Fermi energy. In particular, the increase with energy of the volume integral per nucleon ($[r^2]_V$ in the domain) 10 MeV $<E<0$ MeV is due to the increase of r_V, while the phenomenological analyses would incorrectly ascribe this to an increase of the depth U_V. The energy dependence of r_V may play an important role in the determination of absolute spectroscopic factors from pickup or stripping reactions.[13]

Our approach can also be used to improve the estimate of the influence of the dispersive contribution on the charge and matter-density distribution.[14] In this context it would be of great interest to apply it to the p-^{208}Pb system. In order to do so, one should perform accurate optical-model analyses of the p-^{208}Pb cross sections which are available below 20 MeV[8]; it is important that these new analyses treat the Woods-Saxon parameters

U_V, R_V, and a_V as adjustable. Work on the reanalysis is in progress.[15]

In summary, we have proposed a procedure for the calculation of detailed properties of the shell-model potential for bound nucleons from those of the optical-model potential as determined from analyses of scattering cross sections. This method is based on the dispersion relation which connects the imaginary to the real part of the mean field. This method has been applied to the n-^{208}Pb system. At the Fermi energy our calculation yields the following values for the Woods-Saxon parameters of the shell-model potential, Eq. (1): $U_V = 41.5$ MeV, $r_V = R_V A^{-1/3} = 1.25$ fm, and $a_V = 0.73$ fm. We showed that the coupling between the single-particle and the other degrees of freedom gives rise to a rapid and characteristic energy dependence of the potential radius in the vicinity of the Fermi energy; this reflects the importance of the virtual excitation of the vibrations of the ^{208}Pb core.

Our interest in the relationship between the shell-model and the optical-model potentials has been stimulated and sustained by Professor G. E. Brown.

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