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AN EFFECTIVE SINGLE-PARTICLE POTENTIAL

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Abstract: In the framework of the independent-particle model, we study the scattering function for one particle in the continuum and for $n-1$ particles in bound states. An effective single-particle potential is constructed in such a way that the resulting effective single-particle wave function provides the same scattering matrix. The Pauli principle generates a non-local effective potential which behaves like r^{-2} at the origin. Possible physical consequences are discussed.

1. Introduction

The independent-particle model is the basis of many microscopic descriptions of nuclei. The assumptions that the particles move in a common potential $V(r)$ is motivated by the physical intuition that one particle "feels" all other particles as an average potential. This is formally exhibited in the Hartree-Fock potential [1]) or, in a phenomenological way, in the optical-model analysis of elastic nucleon-nucleus scattering [2]). The only correlation among the particles is, in the framework of the independent-particle model, the exclusion principle. If we take into account the configuration where one particle is in a scattering state, described by $\chi_k^{(+)}$, and where the other $n-1$ particles are in bound states, described by the functions φ_i, then the n-particle wave function is the Slater determinant $\psi_k^{(+)} = \mathscr{A}(\varphi_1(1)\dots\varphi_{n-1}(n-1)\chi_k^{(+)}(n))$.

We consider the scattering amplitude $S(k)$ given by

$$S(k)\delta(E-E') = \langle\psi_k^{(+)}|\psi_{k'}^{(-)}\rangle = \langle\chi_k^{(+)}|\chi_{k'}^{(-)}\rangle. \tag{1.1}$$

The second line of eq. (1.1) follows from the orthogonality of the scattering and bound-state wave functions. Thus, the n-particle problem leads to the same scattering amplitude as the single-particle problem in which only one particle is scattered by the potential $V(r)$ and no other bound particles are present.

We want to replace the familiar n-particle wave function of this problem, which is a Slater determinant, by a single-particle wave function which involves only the nth particle and which does not involve explicitly the remaining $n-1$ bound particles. In other words, we want to replace the potential, in which $n-1$ bound levels are occupied and one particle scatters, by a modified potential in which the mentioned bound-state levels do not exist but the single-particle scattering phase remains unchanged. Formally, we are looking for an effective *single*-particle wave function $\xi_k^{(+)}$ which leads to the n-particle scattering amplitude given by eq. (1.1). The function $\chi_k^{(+)}$ is not acceptable as an effective single-particle wave function for the actual n-particle problem because of the following reason: in a single-particle S-matrix element all poles which arise from poles of the scattering function are interpreted as bound-state poles. The matrix element $\langle\chi_k^{(+)}|\chi_{k'}^{(-)}\rangle$ displays such poles at energies which correspond to already-filled levels of the actual n-particle problem. At such energies, the poles cannot correspond to bound-state poles of the effective single-particle problem. Our aim is to look for an effective single-particle potential and a corresponding wave function $\xi_k^{(+)}$ so that $\langle\xi_k^{(+)}|\xi_{k'}^{(-)}\rangle = \langle\chi_k^{(+)}|\chi_{k'}^{(-)}\rangle$. Those poles which correspond to already filled states should not arise as poles of the function $\xi_k^{(+)}$, so that they are no longer interpreted as bound-state poles. We may also say that within the framework of the independent-particle model we are looking at the "optical potential" which is different from $V(r)$ because of the Pauli principle.

We assume that the original potential $V(r)$ is not singular in the sense that Levinson's theorem holds [3]). The new effective potential must be singular, since, by construction, the phase shifts belonging to it are unchanged, whereas the number of bound states is smaller. In sect. 3, where the properties of the effective potential are discussed, it is shown that there always occurs a repulsion proportional to r^{-2}.

Possible physical consequences of these results are discussed in the last section. The majority of the phenomena in nuclear physics can only be explained by a residual interaction. This goes beyond the scope of the considered model. Whether the extension of this model is reasonable and tractable is still to be investigated. A possible application could concern the description of heavy-ion reactions which would be more satisfactory if the Pauli principle could be taken into account by dynamical assumptions.

2. Construction of the effective single-particle potential

In the following we forget about spin and isospin and only consider a fixed partial wave for the effective single-particle problem. We assume that the given potential $V(r)$ is well behaved so that it furnishes a Jost function $g(k)$ which possesses an analytic continuation into the lower k-plane [3]). Then the poles of the scattering amplitude

$$S(k) = \frac{g(-k)}{g(k)} \tag{2.1}$$

are bound-state poles belonging to the potential $V(r)$ if they are produced by zeros of the Jost function $g(k)$ on the positive imaginary k-axis.

Assume that $g(ia) = 0$ and that the point $k = ia$ corresponds to an energy level which is already filled by one of the remaining particles of the actual n-particle problem. To be consistent this pole may not be interpreted as a bound-state pole of the effective single-particle problem which we are looking for. Therefore, we have to look for a potential which furnishes a Jost function $f(k)$, so that

$$\frac{f(-k)}{f(k)} = \frac{g(-k)}{g(k)}, \tag{2.2}$$

and where $f(ia)$ does not vanish. This implies that $f(k)$ has a pole at $k = -ia$.

From the representation [3])

$$g(k) = \prod \left(1 - \frac{E_n}{E}\right) \exp\left[\frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\delta(k')\mathrm{d}k'}{k-k'}\right], \tag{2.3}$$

we may conclude that

$$f(k) = \frac{k^2}{k^2+a^2}\, g(k) \tag{2.4}$$

is the desired new Jost function. It differs from $g(k)$ by dropping the factor $1-E_n/E$ for $E_n = -a^2\hbar^2/2m$ and it has still the same phase for real k-values.

To construct the potential belonging to the Jost function $f(k)$ given by eq. (2.4) we use a slightly modified version of the method which is described in ch. 14 of Newton's book [3]). Without proof we refer to the formulas which we use in the next section.

From the regular function $\varphi(k, r)$ and the irregular function $f(k, r)$, which are solutions of the Schrödinger equation containing the potential $V(r)$, we form the following expressions:

$$x(k, r) = -\frac{W(\varphi(ia, r), f(k, r))}{k^2+a^2},$$

$$y(k, r) = -\frac{W(\varphi(ia, r), \varphi(k, r))}{k^2+a^2}. \tag{2.5}$$

Thereby $W(f, g)$ denotes the Wronskian $fg'-gf'$. We further introduce

$$K(r) = -\frac{f(0, r)}{x(0, r)}. \tag{2.6}$$

Then the potential

$$U(r) = V(r)+2\frac{\mathrm{d}}{\mathrm{d}r} K(r)\varphi(ia, r) \tag{2.7}$$

furnishes the Jost function

$$g_1(k) = \frac{k}{k-ia}\, g(k),$$

if $g(k)$ is the Jost function belonging to $V(r)$. The new regular and irregular functions are given by

$$\varphi_1(k, r) = \varphi(k, r)+K(r)y(k, r),$$
$$f_1(k, r) = \frac{k+ia}{k}(f(k, r)+K(r)x(k, r)). \tag{2.8}$$

We repeat this procedure once more after having replaced $\varphi(k, r)$ by $\varphi_1(k, r), f(k, r)$ by $f_1(k, r)$ and ia by $-ia$. This provides the potential which leads to the Jost function

$$f(k) = \frac{k^2}{k^2+a^2}g(k).$$

The uniqueness of the resulting local potential will be discussed in the last section of this paper.

3. Properties of the effective single-particle potential

We first investigate the behaviour of the effective potential at the origin. For simplicity we treat only s-waves in detail. Higher partial waves lead essentially to the same results as is outlined later.

The regular solution of the Schrödinger equation containing the potential $V(r)$ has, by definition, the following expansion at the origin

$$\varphi(k, r) = r+a_3(k)r^3+\dots. \tag{3.1}$$

We also need the expansion of the irregular function

$$f(k, r) = g(k)+b_1(k)r+\dots. \tag{3.2}$$

We recall that $g(k)$ is the Jost function which is provided by the potential $V(r)$.

Inserting these expansions into the expressions (2.5), we get the following expansions

$$x(k, r) = \frac{g(k)}{k^2+a^2}+\frac{r^2}{2}g(k)+\dots,$$
$$y(k, r) = \frac{r^3}{3}+\dots. \tag{3.3}$$

To obtain these expressions, use is made of the fact that the functions φ and f obey the Schrödinger equation. From eqs. (2.6) and (2.8) we finally obtain the expansions:

$$\varphi_1(k, r) = r+r^3\left(a_3(k)-\frac{a^2}{3}\right)+\dots,$$
$$f_1(k, r) = \frac{g(k)k}{k-ia}+rA(k)+\dots, \tag{3.4}$$

with

$$A(k) = \frac{k+ia}{k}\left(b_1(k) - \frac{g(k)}{g(0)}\,\frac{a^2 b_1(0)}{k^2+a^2}\right).$$

In order to obtain the potential and the wave functions which provide the Jost function $g(k)k^2/(k^2+a^2)$ we insert the expansions (3.4) into eqs. (2.5) and obtain

$$\begin{aligned} x_1(k,r) &= \frac{k}{k-ia}\,\frac{g(k)}{k^2+a^2} + \frac{r^2}{2}\,\frac{g(k)k}{k-ia} + \frac{r^3}{3}A(k) + \ldots, \\ y_1(k,r) &= \frac{r^3}{3} + \ldots . \end{aligned} \tag{3.5}$$

From the second of eqs. (3.4) and the first of eqs. (3.5), we obtain, using eq. (2.6),

$$K_1(r) = -\frac{rA(0)+\ldots}{\frac{1}{3}r^3A(0)+\ldots}. \tag{3.6}$$

From eq. (2.7) it can be seen that the following additional term arises in the effective potential

$$\begin{aligned} \Delta V(r) &= 2\frac{\mathrm{d}}{\mathrm{d}r}\,K_1(r)\varphi_1(ia,r) \\ &= \frac{6}{r^2} + \ldots . \end{aligned} \tag{3.7}$$

Thus the effective potential is repulsive and singular at the origin.

Let us show that the behaviour of the wave functions $\varphi_2(k,r)$ and $f_2(k,r)$ which are solutions of the corresponding Schrödinger equation is consistent with this result. We insert the expressions (3.4), (3.5) and (3.6) into the l.h.s. of eq. (2.8) and obtain

$$\begin{aligned} \varphi_2(k,r) &= -\frac{k^2}{15}r^3 + \ldots, \\ f_2(k,r) &= -\frac{3}{r^2}\,\frac{g(k)}{k^2+a^2} + \ldots . \end{aligned} \tag{3.8}$$

The powers of r correspond in fact to the behaviour of the potential given by eq. (3.7). The properly normalized regular solution is given by

$$\bar{\varphi}_2(k,r) = -\frac{15}{k^2}\,\varphi_2(k,r).$$

From the representation

$$\bar{\varphi}_2(k,r) = -\frac{15}{2ik(k^2+a^2)}\left(f_2(k,r)g(-k) - f_2(-k,r)g(k)\right),$$

one sees that the zero of the Jost function $f(k) = g(k)k^2/(k^2+a^2)$ at $k = 0$ does not cause a bound state at $k = 0$, since, besides an r-independent factor, the asymptotic behaviour of $\bar{\varphi}_2(0, r)$ is equal to that of $\varphi(0, r)$which was not a bound-state function.

To establish the asymptotic behaviour for large distances of the potential $\Delta V(r)$ given by eq. (3.7), we have to investigate the asymptotic behaviour of

$$\begin{aligned} 2\frac{\mathrm{d}}{\mathrm{d}r} K_1(r)\varphi_1(ia, r) &\approx 2\frac{\mathrm{d}}{\mathrm{d}r} \frac{a^2}{\varphi_1'(ia, r)} \varphi_1(ia, r) \\ &\approx \text{const}\, \mathrm{e}^{-2ar}. \end{aligned} \tag{3.9}$$

To obtain this result, use was made of the relations

$$f_1(k, r) \approx \mathrm{e}^{ikr},$$

$$\varphi_1(k, r) = \left\{ f_1(k, r)\frac{g(-k)k}{k+ia} - f_1(-k, r)\frac{g(k)k}{k-ia} \right\} \Big/ 2ik.$$

We summarize our findings: starting from the S-matrix element $g(-k)/g(k)$ we have constructed the potential and the wave function which provide the same analytic form of the S-matrix element but with a different meaning of the pole at $k = ia$. Instead of the zero of the "old" Jost function $g(k)$, it is a pole of the "new" Jost function $f(k)$ at $k = -ia$ which provides the pole of the S-matrix, thus it is no longer to be interpreted as a bound-state pole but rather as a left-hand singularity. It is the ex-potential tail of the constructed potential which causes this left-hand pole. The violation of Levinson's theorem is connected with the singular behaviour of the potential at the origin.

Coming back to the original n-particle problem, we should consider the possibility that more than only one zero of $g(k)$ corresponds to an already-filled level. Using the same procedure as we did above one can check that the Jost function

$$h(k) = \frac{k^{2s}}{(k^2+a_1^2)\dots(k^2+a_s^2)}\, g(k)$$

provides a potential which still behaves like dr^{-2} at the origin. The constant $d > 0$ increases with increasing number s.

The same holds if we consider higher partial waves. The Jost function

$$f_l(k) = \frac{k^2}{k^2+a_l^2}\, g_l(k)$$

leads to a potential which behaves like cr^{-2} at the origin. The constant c is in general not six as in the discussed s-wave case, but larger. The zero of $f(k)$ at $k = 0$ introduces no bound state at zero energy.

Clearly, the procedure gives rise to different effective single-particle potentials $V_l^{\text{eff}}(r)$ for different values of the angular momentum l. This provides a non-locality in the total potential

$$V^{\text{eff}} = \sum_l \frac{2l+1}{4\pi} P_l(\hat{r}\hat{r}') \frac{\delta(r-r')}{r^2} V_l^{\text{eff}}(r).$$

Similarly, a spin and isospin dependence would occur if we considered these quantum numbers, since for different spin and isospin states different poles of $S(k)$ should be reinterpreted.

4. Example

We illustrate the procedure by considering two particles in a s-wave eigenstate of a square-well potential $V(r) = -V_0\Theta(R-r)$. The first particle is assumed to be in a bound state of the energy $E = -a^2\hbar^2/2m$. Its regular function is given by

$$\varphi(r) = \begin{cases} \dfrac{\sin \kappa_0 r}{\kappa_0} & \text{for} \quad r < R \\ \mathrm{e}^{aR} \dfrac{\sin \kappa_0 R}{\kappa_0} \mathrm{e}^{-ar} & \text{for} \quad r > R, \end{cases}$$

with

$$\kappa_0 = \sqrt{\frac{2m}{\hbar^2} V_0 - a^2}.$$

The second particle is assumed to be in a scattering state. The irregular function is given by

$$f(k, r) = \begin{cases} \dfrac{\mathrm{e}^{ikR}}{\kappa} (\kappa \cos \kappa(R-r) - ik \sin \kappa(R-r)) & \text{for} \quad r < R \\ \mathrm{e}^{ikr} & \text{for} \quad r > R, \end{cases}$$

with

$$\kappa = \sqrt{\frac{2m}{\hbar^2} V_0 + k^2},$$

and the regular function by

$$\varphi(k, r) = \frac{1}{2ik} (f(k, r)g(-k) - f(-k, r)g(k)),$$

where the Jost function $g(k) = f(k, 0)$ is used.

According to our philosophy we look for the potential which provides the scattering function $S(k) = g(-k)/g(k)$ but which does not yield a bound state at $E = -a^2\hbar^2/2m$. We proceed in the manner described in sect. 2. Using the functions given above we obtain as a first step the functions $f_1(0, r)$ and $\varphi_1(i, a, r)$ by eqs. (2.8). Then, using eqs. (2.5), (2.6) and (2.7), the potential which provides the Jost function $f(k) = g(k)k^2/(k^2+a^2)$ is given by

$$U(r) = V(r)+2a^2 \frac{\mathrm{d}}{\mathrm{d}r} \frac{f(0, r)\varphi(r)}{f'\varphi - f\varphi'} + 2a^2 \frac{\mathrm{d}}{\mathrm{d}r} \frac{f_1(0, r)\varphi_1(ia, r)}{f_1'\varphi_1 - f_1\varphi_1'}.$$

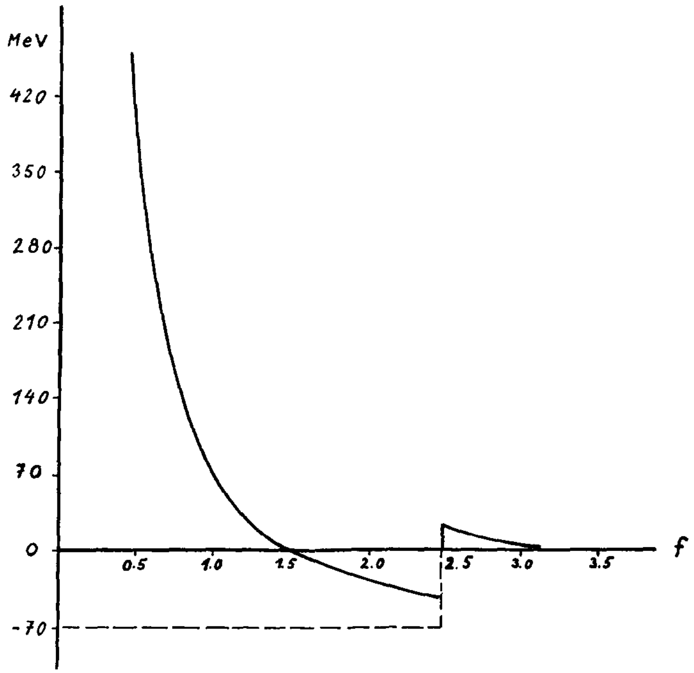

Fig. 1. The potential which provides the same s-wave scattering phase shift as the square well (dashed line) but no bound state.

This potential is shown in fig. 1. We used the parameters $V_0 = 70$ MeV, $E = -45$ MeV and $R = 2.5$ fm. Since the explicit formula is somewhat complicated and of little interest, we do not give it here.

5. Summary and discussion

We have constructed an effective single-particle potential for an n-particle problem in which the only correlation among the particles is the exclusion principle. The effective potential does not provide those bound states which are occupied by the $n-1$ particles of the actual n-particle problem. The scattering phase shift for the nth particle is left unchanged. The levels which are not forbidden for the nth particle by the Pauli principle, correspond to bound-state energies of the effective potential. Let us add some words of the possible physical implication of the model.

Whereas for all energies the asymptotic behavior of the effective scattering wave function $\xi^{(+)}$ is the same as the one of the shell-model wave function $\chi^{(+)}$, the two functions differ at finite distance where the potential is non-vanishing. The effective potential pushes outwards the effective wave function. As a consequence, the effective wave function of those bound states which are still available for the nth particle differ from the shell-model wave function. A shell model 2s state, e.g., would correspond to an effective bound-state wave function with a radial part which looks rather like a shell-model 1d state wave function. Thus, one has to be careful in applying this effective single-particle model for the calculation of matrix elements of single-particle operators [5]). For example, let us consider the matrix element $\langle\varphi_B|H_{EM}|\chi'^{(+)}\rangle$ which is used to describe a (γ, n) process in the framework of the independent-particle model [4]). In the present effective single-particle model one would encounter the expression $\langle\zeta_B|H_{EM}|\xi^{(+)}\rangle$, where ζ_B like φ_B, describes the state from which the neutron escapes, but, as mentioned above, the radial wave functions are quite different. This shows that the physical implications of the effective single-particle potential, introduced here, require a careful examination. Some freedom, however, exists which might be exploited.

Indeed, the local radial effective potential is unique for a given partial wave only if no bound state is available for the nth particle. If the Pauli principle admits N bound levels for the nth particle, then there exists an N-parameter family of potentials [3]). This shows that we would then have the freedom to change the shape of the radial part of the bound-state wave functions, e.g., in order to adjust matrix elements of single-particle operators in which a bound state is involved. The potential which we have constructed is the one with the shortest range. Eq. (3.9) shows that this range is given by the highest level which is forbidden for the nth particle by the exclusion principle. We may compare this exponential tail with the one of an optical-model analysis of elastic nucleon-nucleus scattering [2]) which also has the form $e^{-r/b}$. If the last bound particle has a binding energy of 6, 8 or 10 MeV, we get for b the values 0.9, 0.8 or 0.7 fm, respectively. This corresponds to typical values of the diffuseness b in a Woods-Saxon type analysis [2]).

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