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Scattering phases for particles with nonzero orbital momenta and resonance regimes in the Pais approximation

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Contents

Abstract. The functional Pais equation for scattering phases with nonzero orbital momenta is solved in the case of low-energy particles. For short-range screened potentials, in particular, Yukawa or Thomas–Fermi potentials, the Pais equation is shown to reduce to transcendental equations. For the potentials varying $\sim r^{-n}$, $n > 0$, simple algebraic equations are obtained for determining the phases δ_l, $l \neq 0$. Possible applications of the Pais approximation to the problem of finding resonance regimes in the scattering of low-energy particles with nonzero orbital momenta are discussed.

1. Introduction

Calculating the phases for the scattering of slow particles by a certain potential (for example, atomic) is a basic problem in quantum mechanics, for whose solution standard textbook methods exist (see, for example, Ref. [1]). There are a large number of computational procedures available for numerically determining the δ_l phases as a function of the particle energy k^2 (hereinafter, the units of measure based on the system $\hbar = 2m = 1$, with m being the mass of the particle, are used). The very problem of calculating the δ_l phases with momentum $l \neq 0$ has a reasonable physical meaning when these phases are not small compared with the δ_0 phase. Such a situation arises when some $l \neq 0$ partial amplitudes exhibit resonances.

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On the other hand, problems also exist that require a good approximation for the δ_l phases, regardless of the situation with the resonances. Notice, for example, that δ_l phases enter the Friedel sum rule for alloys, which determines the valence difference or the excess charge of the impurity ion relative to the matrix ions. The same phases are used when calculating the residual resistivity and the Knight shift. Another point to mention is that a change in the Fermi density of states due to impurity atoms in the metal matrix changes the contribution to the heat capacity of the metal. This is directly related to the energy derivative, at the Fermi level, of the scattering phases for the perturbing (impurity) potential. It is well known that localized impurity atoms in a metal lead to charge density oscillations (so-called *Friedel oscillations*) at large distances. The amplitudes and phases of such oscillations are also functions of scattering phases with different momentum l [2].

Finally, it is also important to note that in nuclear scattering problems the phases δ_l are by no means always small. All calculations of this type require that the partial scattering characteristic be available precisely for different l. It is therefore of interest to find relations, valid near the possible resonances, which are suitable for describing scattering phases as functions of collision energy, particle momentum, and potential parameters. In this paper, which is an essential extension and elaboration of work [3], efficient methods for calculating δ_l phases ($l \neq 0$) for slow particles and for identifying possible resonance situations are discussed.

Our starting point is the following functional (relative to the δ_l phase) equation obtained variationally by Pais [4]:

$$\frac{2l+1-2\delta_l/\pi}{2l+1-4\delta_l/\pi}\,\delta_l = -\frac{\pi}{2}\int_0^\infty U(r)\,J^2_{l+1/2-2\delta_l/\pi}(kr)\,r\,\mathrm{d}r\,. \quad (1)$$

Here, $U(r)$ is the potential, and $k^2 = E > 0$ is the particle energy. The variational problem addressed by A Pais was that for the Schrödinger equation on the class of $J_{l+1/2+\lambda}$

functions, where J_μ is the Bessel function of order μ, and the parameter λ turns out to be related with the δ_l phase by the simple formula: $\delta_l = -(\pi/2)\,\lambda$.

We will follow Pais's original work to briefly describe how integro-functional equation (1) is obtained. The procedure is reproduced in a quite clear way in Ref. [5] and is basically as follows. First, we write down the radial Schrödinger equation for a partial wave with momentum $l \neq 0$:

$$(H_l - k^2)\,\Phi_l(r) = 0\,. \tag{2}$$

The Hamiltonian H_l is defined routinely as

$$H_l = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{r^2} + U(r)\,. \tag{3}$$

If $U(r) = 0$, we can write the exact solution as follows:

$$\Phi_l(r) = r^{1/2} J_{l+1/2}(kr)\,. \tag{4}$$

Here, $J_{l+1/2}$ is the Bessel function of half-integer order.

If the potential $U(r)$ is small compared to $l(l+1)/r^2$ for $r \to \infty$, one can attempt to obtain an approximate solution for $l \neq 0$ by taking

$$\Phi_l^{\mathrm{P}}(r) = r^{1/2} J_{l+1/2+\lambda}(kr) \tag{5}$$

as a trial function. The parameter λ is obtained here variationally, and the asymptotics for large r is

$$\Phi_l^{\mathrm{P}}(r) \approx \sin\left[kr - \frac{\pi}{2}\,(l+\lambda)\right]. \tag{6}$$

It is from this that we obtain the relationship $\delta_l = -(\pi/2)\,\lambda$ mentioned above.

Determining λ requires the solution of the equation

$$\int_0^\infty \Phi_l^{\mathrm{P}}(H_l - k^2)\,\Phi_l^{\mathrm{P}}\,\mathrm{d}r = 0\,. \tag{7}$$

It should be noted that, while such a procedure uses the fact that $U(r)$ is small compared to $l(l+1)/r^2$, it places no constraints on the value of the ratio k^2/U, implying that for the given potential the Pais equation should be valid for both large and small particle energies.

Tietz [6, 7] obtained Eqn (1) in a way similar to that used in deriving the usual Born formula. Equation (1) holds for $l \neq 0$. From Pais's derivation, it clearly follows that the scattering phase should be normalized so as to satisfy the inequality $\delta_l < (\pi/2)(l+1)$. Tietz showed that equation (1) adequately describes the scattering of a neutron by a proton for neutron energies larger than the depth of the equivalent potential well. At the same time, equation (1) should work much better in the opposite limiting case of $E < |U|$ (see Ref. [8]). An example clearly illustrating this point is given in Section 3. An important feature of equation (1) is the presence of the δ_l phase in the order of the Bessel function under integral. This prevents functional equation (1) from being analytically solvable for cases other than special ones and possibly explains, to some extent, why the Pais approximation was forgotten and not used for a long time — not even by Pais himself in its originally intended field of nuclear particle scattering.

The scattering of slow particles presents a different situation, in which equation (1) can be solved for a fairly wide class of potentials, including the screened Coulomb potential, power-law potentials, and various combinations of power-law and exponential varieties. For the variational derivation of equation (1) to be correct, it is necessary that, as $r \to \infty$, the potential $U(r)$ approach zero as fast as or faster than the centrifugal potential $l(l+1)/r^2$. It is the requirement which, in essence, specifies the condition for the validity of equation (1). In this context, there are clearly no strict constraints on the short-range potentials actually dealt with in the theory of elementary processes or in solid-state pseudopotential calculations. Corresponding formulas can also be obtained for the analytically approximated Thomas–Fermi potential.

The interesting and informative work [5] addressed whether the Pais equation allows solutions for particles other than slow ones. It is easily verified that our results for the corresponding potentials (including those in Ref. [3]) can also be obtained by taking the limit of the formulas of Ref. [5] for small particle energies. Still, it is precisely the scattering of slow particles that can produce resonance situations and which we therefore consider the most important.

How such resonances arise can be qualitatively understood, for example, by recognizing that effectively increasing the depth of a potential well produces in it new levels with certain l values. These have a near 'zero' energy, which is precisely when scattering resonances can occur.

Such a situation, characteristically encountered in developing the theory of atomic electron shells (as the nuclear charge Z increases), is well described by, for example, the Thomas–Fermi model (see Ref. [1]). Frequently used in nuclear physics research is the Woods–Saxon potential (see Section 4); changes in its parameters are also likely to be due to the appearance of new levels and, hence, to scattering resonances (shell and optical models of the nucleus). The Pais approximation enables calculating fairly accurately the scattering of slow particles, thus allowing energy estimates for the newly emerging shallow levels. No systematic (let alone analytical) comparisons appear to have been made for various potentials for the energies of such levels and for the parameters of $l \neq 0$ resonances.

In fact, the solution to the inverse problem — which is to find the relationship between the potential parameters and the energy of the scattered particle, assuming the existence of a resonance with a specific value of l — is also within the reach of the Pais approximation. This question is discussed in Section 6, where a method for constructing 'resonance' curves is also presented.

2. Pais approximation approach to calculating scattering phases for slow particles with nonzero momenta

The examples discussed below allow us to state that, in many cases, the Pais approximation effectively works better than the Born approximation, and sometimes the latter even fundamentally fails and should be replaced by the former. Therefore, it is of interest, both practically and methodologically, to be able to construct analytical formulas for the scattering phases or to reduce complex integro-functional equation (1) to simple transcendent or algebraic equations.

2.1 Rectangular well potential

The first example is the potential

$$U(r) = \begin{cases} -U_0\,, & r < a\,, \\ 0\,, & r > a\,. \end{cases} \tag{8}$$

The Bessel function squared appearing in the integrand of Eqn (1) can be expanded in a series as [9]

$$J_\mu^2(z) = \sum_{n=0}^{\infty} \frac{(-1)^n\,\Gamma(2\mu+2n+1)(z/2)^{2\mu+2n}}{n!\left[\Gamma(\mu+n+1)\right]^2\Gamma(2\mu+n+1)}\,, \tag{9}$$

where $z = kr$, $\Gamma(x)$ is the gamma function, and $\mu = l + 1/2 - 2\delta_l/\pi$. Accounting for the boundedness of potential (8), expansion (9) can, for sufficiently small energies k^2, be restricted to the first term, resulting, after evaluating the integral in Eqn (1) and doing some elementary algebra, in the following formula

$$\Phi_1(l,s) = (U_0 a^2)(ka)^{2s-1}\,, \tag{10}$$

where

$$\Phi_1(l,s) = \frac{2^{2s-1}(l+s)(l-s+1)(2s+1)\left(\Gamma(s+1/2)\right)^2}{2s-1}\,, \tag{11}$$

$$s = \mu + \frac{1}{2} = l + 1 - \frac{2\delta_l}{\pi}\,. \tag{12}$$

Equation (10) determines, for given l, k^2, and the potential parameters (U_0 and a), the linear-in-phase-δ_l quantity s. Expansion (9) can also be of benefit in other cases, in which more of its terms are included.

2.2 Yukawa and Thomas–Fermi potentials

As a second example, let us consider the Yukawa potential

$$U(r) = -\exp(-\lambda r)\,\frac{Z}{r}\,. \tag{13}$$

The integral $I = Z\int_0^\infty \exp(-\lambda r)\,J_\mu^2(kr)\,\mathrm{d}r$ in formula (1) is expressed in terms of the Legendre function of the second kind to give

$$I = \frac{Z}{\pi k}\,Q_{l-(2\delta_l/\pi)}\left(\frac{\lambda^2+2k^2}{2k^2}\right). \tag{14}$$

In our case of small energies, it is assumed that $\lambda^2/k^2 \gg 1$. The corresponding asymptotic form of the Legendre function $Q_\nu(\xi)$, when

$$\xi = 1 + \frac{\lambda^2}{2k^2} \gg 1\,, \quad \nu = l - \frac{2\delta_l}{\pi} = \mu - \frac{1}{2}\,,$$

can be obtained by using the Laplace integral representation of this function in the complex plane [10]:

$$Q_\nu(\xi) = \int_0^\infty \frac{\mathrm{d}\psi}{\left[\xi + (\xi^2-1)^{1/2}\cosh\psi\right]^{\nu+1}}$$

(for noninteger ν, the cut along the real axis runs from $\xi = -\infty$ to $\xi = +1$; if $\nu = n > 0$ is an integer, the cut along the same axis extends from $\xi = -1$ to $\xi = +1$). For real $\xi \gg 1$, one has

$$Q_\nu(\xi) = \frac{2}{(2\xi)^{\nu+1}}\int_0^\infty \frac{\mathrm{d}\psi}{(\cosh\psi)^\rho}\,, \quad \rho = 2(\nu+1)\,.$$

The last integral is expressed in terms of the beta function. The asymptotics of formula (14) we are concerned with can now be written, after some standard transformations, as

$$I = \frac{Z}{\sqrt{\pi}k}\left(\frac{k^2}{\lambda^2}\right)^s \frac{\Gamma(s)}{\Gamma(s+1/2)}\,. \tag{15}$$

The parameter s is defined as above by formula (12). The equation determining s (and hence the phase δ_l) can now be written down as

$$\frac{(l+s)(l+1-s)}{2s-1} = \frac{Z}{\sqrt{\pi}k}\left(\frac{k^2}{\lambda^2}\right)^s \frac{\Gamma(s)}{\Gamma(s+1/2)}\,. \tag{16}$$

The constant λ can be chosen such that the Yukawa and Thomas–Fermi potentials have the same asymptotics

$$\frac{Z}{r}\,\chi\left(\frac{rZ^{1/3}}{b}\right) \sim \frac{Z}{r}\exp(-\lambda r) \text{ as } r \to 0\,,$$

where χ is the Thomas–Fermi functions, $\lambda = \lambda_0 Z^{1/3}$, $b = 0.885$, and $\lambda_0 \approx 1.8$. Carrying the factors dependent on s alone to the left-hand side of formula (16) yields the relation [cf. Eqn (10)]

$$\Phi_2(l,s) = Z^{2/3}\left(\frac{k}{Z^{1/3}}\right)^{2s-1}. \tag{17}$$

A simple procedure exists in which the calculation of s from Eqn (10) or Eqn (17) can be reduced to nomogram work. The last formula will serve to illustrate this procedure. After taking the logarithm of formula (17), the left- and right-hand sides of the equality contain the function $y_1(s) = f(l,s)$ and an expression of the form $A(Z) + B(k,Z)(2s-1) = y_2(s)$, respectively. For each l, it is possible to tabulate $y_1(s)$ and to construct a series of corresponding curves in the (s, y) plane. Then, fixing the parameters Z and k, and plotting straight lines $y_2(s)$ in the same plane, it is an easy matter to find the intersection points of $y_1(s)$ and $y_2(s)$. If such a point is $s = s_0$, then $\delta_l = (\pi/2)(l+1-s_0)$ for given (l, k, Z). (Notice that the phases δ_l are not assumed to be small.) If $\delta_l \ll 1$, we have

$$\delta_l \sim D_l Z^{2/3}\left(\frac{k}{Z^{1/3}}\right)^{2l+1}\,,$$

as it must according to the general rules of quantum mechanics (D_l is a constant dependent on l).

In perfect analogy to the procedure just outlined is that used to calculate scattering phases for the model potential

$$U(r) = -(1+\beta r^{3/2})\exp(-\alpha r)\,\frac{Z}{r} \tag{18}$$

with $\beta = 4/3Z^{1/2}b^{-3/2}$, $\alpha = 1.59Z^{1/3}/b$, and $b = 0.885$. In the limit as $r \to 0$, this potential also goes over to the Thomas–Fermi counterpart. The result of calculations for $(k^2/Z^{2/3}) \ll 1$ and $\delta_l < (\pi/2)(l+1)$ (the latter inequality is, in fact, a consequence of the $r = 0$ boundary condition for the wave function) takes the form [3]

$$\begin{aligned} I &= \int_0^\infty (1+\beta r^{3/2})\exp(-\alpha r)\,J_\mu^2(kr)\,\mathrm{d}r \\ &= \frac{1}{\lambda_0^{2s}}\,k^{2s-1}Z^{1-(2/3)s}\,\frac{\Gamma(s)}{\Gamma(s+1/2)} \\ &\quad\times\left\{\frac{1}{\sqrt{\pi}} + \frac{\beta_0}{\lambda_0^{3/2}2^{2s}}\,\frac{\Gamma(2s+3/2)}{\Gamma(s)\,\Gamma(s+1/2)}\right\}, \end{aligned}$$

with $\lambda_0 = 1.59/b$, and $\beta_0 = 4/3b^{-3/2}$. Similar to formula (17), we obtain

$$\Phi_3(l,s) = Z^{2/3}\left(\frac{k}{Z^{1/3}}\right)^{2s-1}. \tag{19}$$

While the specific form of function $\Phi_i(l, s)$ is, of course, determined by the potential itself, for each class of potentials function $\Phi_i(l, s)$ constitutes a universal function of the argument s, which is the exact reason why the calculation of the δ_l phases reduces to elementary operations in the (s, y) plane.

There is another problem that can be solved basically using formulas like those obtained above: to find those potentials (in the specified class!) which produce a resonance level for a particle with momentum l and a given energy experiencing scattering by the potential. For the model potentials considered, this problem reduces to that of finding Z such that, for a given energy k^2, the phase δ_l is exactly or approximately equal to $(\pi/2) \bmod \pi$. The fact that $l \neq 0$ scattering differs from $l = 0$ scattering by the presence of a centrifugal potential barrier readily suggests that a resonance level can, in principle, be quasidiscrete, i.e. positive, as well.

3. Power-law potentials and comparison with the quasiclassical approximation

Of particular interest are scattering potentials of the form $U(r) = -\alpha/r^n$. We will illustrate this by considering the important case of the so-called polarization potential, with $n = 4$. As we will see below, calculations for slow particles using the Pais method lead to values of the δ_l phases known from the exact solution (for the potential $\sim r^{-4}$, the solution of the Schrödinger equation is expressed in terms of Mathieu functions [11]).

The integral on the right-hand side of equation (1) can be considered as the Mellin transform of the corresponding integrand function. The condition for applying the Mellin transform, $\delta_l < (\pi/2)(l - 1/2)$, is somewhat more restrictive than in the examples above: it always holds true for $\delta_l \ll 1$ $(l \neq 0)$, and for $l > 1$ it is also valid for $\delta_l \sim 1$ (note that the phases are found modulo π). Calculating the Mellin transform for the potential $U(r) = -\alpha/r^4$, we obtain for small energies $(\alpha k^2 \ll 1)$:

$$\left[\left(l + \frac{1}{2}\right)^2 - \mu^2\right](\mu^2 - 1) = \frac{\alpha k^2}{2}\,, \tag{20}$$

instead of equation (1), where, as before, $\mu = l + 1/2 - 2\delta_l/\pi$. Equation (20) is simply a quadratic equation in μ^2. The scattering phases for $l = 1, 2, 3, 4, 5, \ldots$ have the respective forms

$$\delta_1 = \frac{\pi\alpha k^2}{1 \cdot 3 \cdot 5}\,, \quad \delta_2 = \frac{\pi\alpha k^2}{3 \cdot 5 \cdot 7}\,, \quad \delta_3 = \frac{\pi\alpha k^2}{5 \cdot 7 \cdot 9}\,,$$
$$\delta_4 = \frac{\pi\alpha k^2}{7 \cdot 9 \cdot 11}\,, \quad \delta_5 = \frac{\pi\alpha k^2}{9 \cdot 11 \cdot 13}\,, \ldots .$$

An entirely similar result follows from the exact (for small αk^2) formula [11]

$$\delta_l = \frac{\pi\alpha k^2}{8(l + 3/2)(l + 1/2)(l - 1/2)}\,. \tag{21}$$

It should also be noted that similar results are obtained for powers $n \neq 4$. For example, for $n = 6$ and $\tilde{\alpha} k^4 \ll 1$ (potential $U(r) = -\tilde{\alpha}/r^6$), the formulas for the phases have the following structure:

$$\delta_l = \frac{3\tilde{\alpha}\pi k^4}{16(2l + 1)(l^2 + l - 15/4)(l^2 + l - 3/4)}\,. \tag{22}$$

The equation that leads to formula (22) has the form

$$\left[\left(l + \frac{1}{2}\right)^2 - \mu^2\right](\mu^2 - 4)(\mu^2 - 1) = \frac{3}{8}\,\tilde{\alpha} k^4\,, \tag{23}$$

which results from the Mellin transform. The asymptotics of Eqn (22) for $l \gg 1$ is as follows:

$$\delta_l \approx \frac{3}{32}\,\frac{\pi\tilde{\alpha} k^4}{l^5}\,. \tag{24}$$

Comparing expression (24) with the known quasiclassical formula reveals that they are identical. Formula (22) [as well as formula (21)] can, in a sense, be considered an accuracy-enhanced version of the quasiclassical result.

It is interesting to note that, by formally comparing formulas like (22) for some potentials with the Born approximation, it is hopefully possible, using the Pais method, to construct for the phases δ_l 'interpolation' formulas valid for not too small energies as well — all the more so given that equation (1) can be considered a 'generalization' of the Born formula. It is very tempting to be able to have the phases 'interpolated' between the regions of applicability of the quasiclassical and Born approximations. However, the corresponding rigorous results are difficult to obtain analytically, and instead the numerical simulation of specific problems is required.

4. Scattering by the Woods–Saxon nuclear potential

Compared to the simple rectangular well or the harmonic oscillator potential, the Woods–Saxon potential, the third most discussed in nuclear physics, is more accurate in describing scattering on atomic nuclei. For light nuclei (with mass number $A \approx 10$), the latter is closer to the oscillator potential, and for heavy ones ($A \approx 200$), to the rectangular well [12].

Let is discuss the particle scattering by the Woods–Saxon potential in the framework of the Pais approximation. Notice that this potential looks like a rectangular well but has its right edge smeared. Let us change the notation of Section 2.1 such that a now denotes the degree of smearing of the potential right edge, and R is the effective radius of the potential. Then we can write down the expression for the potential discussed in the form

$$U(r) = -\frac{U_0}{1 + \exp\left[(r - R)/a\right]}\,. \tag{25}$$

Notice that variations in the parameters of the potential may be due to the appearance of new nuclear levels. Resonance situations could be found by varying not only the potential itself but also the energy of the particle undergoing scattering.

Applying the Pais equation (1) and again using expansion (9) (with only the first term retained in view of the $U(r)$ potential boundedness), the calculation of the right-hand side of equation (1) reduces to evaluating the integral

$$\int_0^\infty \frac{z^{2\mu+1}\,\mathrm{d}z}{1 + \exp\left[(z - z_0)/t\right]}\,, \tag{26}$$

with $z = kr$, $z_0 = kR$, and $t = ka$.

It should be noted that this type of integral is encountered in, for example, statistical physics in calculating the heat

capacity of a degenerate electron gas [13]. Using the formulas of monograph [13], we obtain (adapting the notation) the following asymptotic series expansion:

$$\int_0^\infty \frac{z^{2\mu+1}\,\mathrm{d}z}{1+\exp\left[(z-z_0)/t\right]} = \frac{1}{2\mu+2}\,z_0^{2\mu+2} + \frac{\pi}{6}\,t^2(2\mu+1)\,z_0^{2\mu} + \frac{7\pi^4}{360}\,t^4(2\mu+1)\,2\mu(2\mu-1)\,z_0^{2\mu-2} + \ldots . \quad (27)$$

All further terms in formula (27) can be neglected.

As a result, the right-hand side of the starting equation (1) becomes

$$\frac{\pi}{2}\,\frac{U_0 a^2}{\left(\Gamma(\mu+1)\right)^2}\left(\frac{z_0}{2}\right)^{2\mu}\left[\frac{1}{2\mu+2}\left(\frac{R}{a}\right)^2 + \frac{\pi^2}{6}\,(2\mu+1) + \frac{7\pi^4}{360}\,(2\mu+1)(2\mu)(2\mu-1)\left(\frac{a}{R}\right)^2\right].$$

Returning again to expressions in terms of l and $s = l + 1 - 2\delta_l/\pi$ (recall that $\mu = l + 1/2 - 2\delta_l/\pi$), we arrive at

$$\frac{(l+s)(l-s+1)\left(\Gamma(s+1/2)\right)^2}{2s-1} = U_0 a^2\left(\frac{z_0}{2}\right)^{2s-1} \times\left[\frac{(R/a)^2}{2s+1} + \frac{\pi^2}{6}\,2s + \frac{7\pi^4}{360}\,2s(2s-1)(2s-2)\left(\frac{a}{R}\right)^2\right]. \quad (28)$$

For $a/R \ll 1$, expression (28) reduces to the similar formula for the rectangular well potential:

$$\frac{(l+s)(l-s+1)(2s+1)\left(\Gamma(s+1/2)\right)^2}{(2s-1)\,U_0 R^2} = \left(\frac{kR}{2}\right)^{2s-1}. \quad (29)$$

In formula (28) we can also make the replacements $z_0 \to kR$, $U_0 a^2 \to U_0 R^2 (a/R)^2$, making the limiting transition from Eqn (28) to Eqn (29) for $a/R \ll 1$ totally transparent. It is now totally clear that Eqn (28) differs from Eqn (29) by corrections related to the finite nature of the ratio a/R. However, these formulas are structurally similar, allowing the application to formula (28) of the procedure, described above, of taking the logarithm and finding the scattering phases δ_l for fixed parameters (l, k, U_0, a, R).

5. Obtaining quantitative estimates and some other applications of the Pais approximation

Reference [5] compares the Pais approximation scattering phases with the 'exact' phases obtained by numerically solving the Schrödinger equation for partial waves for a number of potentials.

For example, for the Yukawa potential

$$U(r) = \lambda\left(\frac{R}{r}\right)\exp\left(-\frac{R}{r}\right),$$

with the parameters $\lambda = -10.6$ keV, $R = 0.109 \times 10^{-8}$ cm, and $k = 151.36 \times 10^8$ cm^{-1} (k^2 is the particle energy), the appropriate difference does not exceed 2.3% for $l = 4, 6, 8$, but reaches 12.6% for $l = 2$. Because the collision energy here is not too small, it is reasonable to compare the 'exact' phases with those in the Born approximation. Here, the difference for $l = 4, 6, 8$ varies from 2.5% to 3.9%, and for $l = 2$ it equals 3.5%.

Analysis of tabulated and graphical results [5] for the Thomas–Fermi, Gauss, and Woods–Saxon potentials suggests that the Pais approximation is quite satisfactory in describing scattering, and the larger l, the more close to an exact result is the Pais phase.

Another example is given in Section 3. For the polarization potential $U(r) = -\alpha/r^4$, $\alpha > 0$, even for small phases and for all $l = 1, 2, \ldots$, the Pais phases are coincident with the exact ones (for small αk^2) given by formula (21). For the $U(r) = -\tilde{\alpha}/r^6$ potential, the δ_l phases provide a correct asymptotic behavior for $l \gg 1$ (formulas (22) and (24), where $\tilde{\alpha}k^4$ and the corresponding phases are small).

Additional relevant and useful information can be obtained by calculating the derivatives of the Pais phases with respect to the parameters l, k, R, and s (or μ) [the definition of s and μ is given by formula (12)].

Reference [5] reports the results of such calculations for some potentials. Although these results are unfortunately somewhat unwieldy, they are written down ultimately in terms of special (and hypergeometric) functions and are suitable for performing numerical computations over a wide range of parameters (for example, energy). The derivatives of the scattering phases enter some sum rules in the problems listed in the Introduction and for this reason alone are important.

In some cases, it proves convenient to utilize recurrent relations for special functions, in terms of which the derivatives of the phases are expressed.

Reference [14] provided further development of the Pais approximation and of some of its modifications by addressing the important case with a combination of short-range and Coulomb potentials. It turns out that the modified Pais approximation is quite successful in this case, as well.

Other applications of the Pais approach are also discussed in Ref. [14], among which are scattering of particles in chemical physics problems (complex model potentials), scattering by repulsion potentials, and scattering in gravitational fields of Schwarzschield and Kerr black holes

Analysis shows that Pais phases are closer to the 'exact' ones for repulsion than for attraction potentials. The reason is that (taking into account the centrifugal contribution) the effective potential for repulsion is always nonnegative.

What makes paper [14] especially meritorious is a fairly complex apparatus of Pais–Coulomb functions, which it developed and which enables a number of new problems to be solved, among them those in the presence of resonance situations.

In Section 6, however, we will return again to more elementary questions and discuss resonance situations using a potential well as an example.

6. Resonance situations and resonance curves in the Pais approximation

In this section, we will consider a formal procedure in which resonances can possibly arise due to the scattering of zero-momentum particles on a spherical symmetric rectangular well of finite but sufficiently large depth. We will follow Section 2.1 in denoting the radius of the well as a.

In equation (1) for potential (8), the upper limit of the integral is a, $U(r) = -U_0 = \text{const}$, and the integration can be performed using the well-known formula [10]

$$\int_0^a J_\mu^2(kr)\,r\,\mathrm{d}r = \frac{a^2}{2}\left(J_\mu^2(ka) - J_{\mu-1}(ka)\,J_{\mu+1}(ka)\right). \quad (30)$$

In our case, the relationship $\mu = l + 1/2 - 2\delta_l/\pi$ holds, and the particle energy k^2 is no longer assumed to be in any sense small.

By a resonance situation we formally mean one in which the δ_l phase assumes the value of $\pi/2 + \pi n$, $n \in N_0 = \{0, 1, 2, \ldots\}$. Here, we take account of the condition that the scattering phase for the attraction potential be nonnegative.

It is known that the total scattering cross section for a particle of energy k^2 is given by

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l \,, \tag{31}$$

and that the partial scattering cross section for a particle with a given orbital momentum l is $\sigma_l = (4\pi/k^2)(2l+1) \sin^2 \delta_l$. We do not consider the case of s ($l = 0$) scattering. Therefore, if we ask what the maximum possible value of the partial cross section (at resonance) with $l \neq 0$ is, the answer will be for $\sigma_l = \sigma_{l\,\max} \sin^2 \delta_l = 1$ and $\delta_l = \pi/2 + \pi n$, $n \in N_0$.

In order for the integral on the right-hand side of equation (1) to converge, the order of the Bessel function should be non-negative, and hence

$$\delta_l < \frac{\pi}{2}\left(l + \frac{1}{2}\right). \tag{32}$$

The resonance phases that are, in principle, possible can be written as the following sequence

$$\left\{(2m-1)\,\frac{\pi}{2}\,,\ m = 1, 2, 3, \ldots\right\} = \left\{\frac{\pi}{2}\,,\ \frac{3\pi}{2}\,,\ \frac{5\pi}{2}\,,\ \ldots\right\}.$$

We shall call the number m of a member of this sequence the 'type' of a resonance. For each 'partial wave' which is labelled by the value of the momentum l, inequality (32) yields the admitted types of resonances. It turns out that for $l = 1$ and $l = 2$, the possible resonance type is 1 (i.e. $\delta_l = \pi/2$); for $l = 3$ and $l = 4$, the possible resonance types are 1 and 2 ($\pi/2$ and $3\pi/2$); for $l = 5$ and $l = 6$, the possible resonance types are 1, 2, and 3 ($\pi/2$, $3\pi/2$ and $5\pi/2$), etc.

The types of possible resonances increase in number with increasing l, but for each finite set $m = 1, 2, \ldots, m_0$, exactly two 'partial waves' exist with a maximum allowed identical m_0.

What we consider next is, in a sense, a certain inverse problem: for each l, we substitute allowed values of resonance phases into the Pais equation and find the relation between the parameters $U_0 a^2$ and ka at these resonances.

In a natural way, one can plot the parameter $U_0 a^2$ of a family of wells as a function of ka for different l and for different resonance types. We will call these plots resonance curves.

Simple examples of calculations in like manner follow.

(1) Let $l = 1$. In this case, only the first type of resonance, $\delta_l = \pi/2$, is possible.

In the calculations below, we take advantage of expression (30) and the recurrent formula [10]

$$J_{\nu-1}(z) + J_{\nu+1}(z) = \frac{2\nu}{z}\, J_\nu(z)\,. \tag{33}$$

The Pais equation takes the form

$$1 = \frac{U_0}{2} \int_0^a J_\nu^2(kr)\, r\, \mathrm{d}r\,, \quad \nu = \frac{1}{2}\,,$$

and in view of Eqn (30), one finds

$$\frac{4}{U_0 a^2} = J_{1/2}^2(ka) - J_{-1/2}(ka)\, J_{3/2}(ka)\,. \tag{34}$$

Take into consideration that

$$J_{1/2}(z) = \sqrt{\frac{2}{\pi z}}\, \sin z\,, \quad J_{-1/2}(z) = \sqrt{\frac{2}{\pi z}}\, \cos z\,.$$

From Eqn (33) it follows that

$$J_{3/2}(z) = \frac{1}{z}\sqrt{\frac{2}{\pi z}}\, \sin z - \sqrt{\frac{2}{\pi z}}\, \cos z\,,$$

which, when substituted into Eqn (34), yields ($z = ka$)

$$\frac{4}{U_0 a^2} = \frac{1}{\pi ka}\left(2 - \frac{\sin 2ka}{ka}\right). \tag{35}$$

The asymptotic behavior of $U_0 a^2$ as a function of ka is easily found to be

$$U_0 a^2 = \frac{3\pi}{ka} \quad \text{for} \quad ka \ll 1\,,$$

$$U_0 a^2 = 2\pi ka \quad \text{for} \quad ka \gg 1\,.$$

Clearly, the curve has a minimum and if, for fixed $U_0 a^2$, one draws a horizontal straight line $U_0 a^2 = \text{const}$ above the minimum, the intersection points determine the resonance parameters ka for such a fixed class of wells.

(2) Now let $l = 2$. As with $l = 1$, only the first resonance type, $\delta_l = \pi/2$, is possible.

The Pais equation in this case is written as

$$\frac{4}{3} = U_0 \int_0^a J_{3/2}^2(kr)\, r\, \mathrm{d}r\,.$$

Performing the integration yields

$$\int_0^a J_{3/2}^2(kr)\, r\, \mathrm{d}r = \frac{a^2}{2}\left[J_{3/2}^2(ka) - J_{1/2}(ka)\, J_{5/2}(ka)\right].$$

Let us write out the Bessel functions involved here. These are again expressed in terms of $\sin z$, $\cos z$, and powers of z:

$$J_{3/2}(z) = \frac{1}{z}\sqrt{\frac{2}{\pi z}}\, \sin z - \sqrt{\frac{2}{\pi z}}\, \cos z\,,$$

$$J_{1/2}(z) = \sqrt{\frac{2}{\pi z}}\, \sin z\,,$$

$$J_{5/2}(z) = \sqrt{\frac{2}{\pi z}}\left\{\left(\frac{3}{z^2} - 1\right) \sin z - \frac{3}{z}\, \cos z\right\}.$$

The function $J_{n+1/2}(z)$ for integer n is calculated by consecutively applying formula (33) or by using the general formula known from the theory of Bessel functions:

$$J_{n+1/2}(z) = (-1)^n\, z^{n+1/2} \sqrt{\frac{2}{\pi}} \left(\frac{1}{z}\,\frac{\mathrm{d}}{\mathrm{d}z}\right)^n \left(\frac{\sin z}{z}\right).$$

Using elementary algebra, the Pais equation finally becomes

$$\frac{4}{3U_0 a^2} = \frac{1}{\pi ka}\left[1 + \frac{\sin ka \cos ka}{ka} - \frac{2\sin^2 ka}{(ka)^2}\right]. \tag{36}$$

The asymptotic behavior of Eqn (36) in two limiting cases is

$$U_0 a^2 = \frac{30\pi}{(ka)^3} \quad \text{for} \quad ka \ll 1\,,$$

$$U_0 a^2 = \frac{4}{3}\,\pi ka \quad \text{for} \quad ka \gg 1\,.$$

The resonance parameters ka are found in the class of potentials with a fixed $U_0 a^2$, as was the case with $l = 1$.

An important point to note when working in the space of resonance points is that it is not only different (l, m) pairs but also real resonances in different potential wells may correspond to the possible intersection of resonance curves at the point $(U_0 a^2,\ ka)$. The reason is that the condition $U_0 a^2 = \text{const}$ corresponds not to separate potential wells but to an entire class of sufficiently deep spherical rectangular wells.

Below, we present general expressions for the asymptotics of resonance curves for $ka \ll 1$ and $ka \gg 1$ for any (l, m) pairs. We shall also give a simple rule for finding the intersection points of resonance curves in the $(U_0 a^2, ka)$ plane.

The asymptotic behavior of resonance curves for $ka \ll 1$ and $ka \gg 1$ for a rectangular well potential is uncovered directly from equations (1) and (30). Because the situation under discussion deals with a resonance, we let $\delta_l = (2m-1)\,\pi/2$, $l + 1/2 - 2\delta_l/\pi = \mu = l + 3/2 - 2m > 0$, $z = ka$. Next, we calculate the left-hand side of equation (1). The integral in equation (1) containing the square of the Bessel function will be evaluated using formula (30) and substituting to it the $z \to 0$ asymptotic values:

$$J_\nu(z) = \frac{(z/2)^\nu}{\Gamma(\nu+1)}\,,$$

$\nu = \mu - 1, \mu, \mu + 1$. This asymptotic behavior follows directly from the definition of the Bessel function [10]

$$J_\mu(z) = \sum_{k=0}^{\infty} \frac{(-1)^k (z/2)^{2k+\mu}}{k!\,\Gamma(k+\mu+1)}\,.$$

After some elementary manipulations with a simple expression containing a gamma function, we obtain

$$U_0 a^2 (ka)^{2\mu} = \varphi(l, m)\,, \tag{37}$$

$\mu = l + 3/2 - 2m$. The function $\varphi(l, m)$ can be calculated in a straightforward and accurate way. (The result, though, is somewhat too cumbersome to display here.) Thus, formula (37) provides the asymptotic behavior of a resonance curve for $ka \ll 1$. The asymptotics of the resonance curve for $ka \gg 1$ is obtained in a similar manner.

Having evaluated integral (30), we can substitute into it the asymptotics

$$J_\nu(z) = \sqrt{\frac{2}{\pi z}}\,\cos\left(z - \frac{\pi\nu}{2} - \frac{\pi}{4}\right)$$

for $z \to \infty$. As above, $\nu = \mu - 1, \mu, \mu + 1$.

The Pais equations in this case can be written down in a perfectly simple form

$$\frac{2l + 1 - 2\delta_l/\pi}{2l + 1 - 4\delta_l/\pi}\,\delta_l = \frac{\pi}{2}\,\frac{U_0 a^2}{\pi ka}\,.$$

Making the replacement $\delta_l \to (2m-1)\,\pi/2$, we finally obtain

$$U_0 a^2 = \pi ka\,\frac{2(l+1-m)(2m-1)}{2l+3-4m}\,. \tag{38}$$

This is exactly the required asymptotics of the resonance curve for $ka \gg 1$.

The final point that remains to be discussed is how to find the possible intersection points of the resonance curves. Computer analysis shows that such intersection points are not at all something exotic. Let us assume that different resonance curves intersect in the $(U_0 a^2, ka)$ plane. Let us draw though the intersection point a horizontal straight line corresponding to the class of potentials with a fixed parameter $U_0 a^2$. Let us then write down the Pais equations for these curves assuming, in doing so, that they are specified by the pairs of numbers $(l,\ m)$ and $(\tilde{l},\ \tilde{m})$, respectively. The integrals on the right-hand side of equation (1) are again taken using formula (30). We then arrive at a system of equations, the first of which is

$$\frac{2(l+1-m)(2m-1)}{2l+3-4m} = \frac{U_0 a^2}{2}\left\{J_\mu^2(ka) - J_{\mu-1}(ka)\,J_{\mu+1}(ka)\right\}.$$

The second equation has the same form to within the replacements $l \to \tilde{l}$, $m \to \tilde{m}$, $\mu \to \tilde{\mu}$.

Dividing these two equations by one another, we obtain an equation for determining the parameter ka at the intersection point of the resonance curves. After calculating the corresponding ka, its value can be substituted into any of the two starting equations to determine the value of $U_0 a^2$ at the intersection point. While this essentially elementary procedure requires numerical computations, it gives a conclusive answer as to whether different resonance curves can intersect. Situations in which resonance curves do not intersect are, of course, also possible.

7. Conclusions

It may come as a surprise that in the phase theory of scattering in quantum physics, undoubtedly a 'classical' field of study, problems still arise that can and need to be solved. These include, in particular, finding scattering phases for particles with nonzero momenta in the vicinity of possible resonances. Clearly, this implies computational methods that go beyond the Born approximation which does not at all allow analyzing resonance situations in higher partial waves.

The Pais approximation and the Pais integro-functional equation for calculating phases δ_l (including those for resonance cases) are unfortunately little known to specialists and to teachers in quantum mechanics. It is with this recognition that we thought it worthwhile to write this paper and to highlight the new possibilities that are emerging in this field.

Notice once again that, in our view, a very important problem still remains unsolved: that of the relationship between shallow bound states and the appearance of resonances in the scattering of low-energy particles (with $l \neq 0$). Still, ideas about the existence of this relationship have been around in the serious scattering theory literature (see, for example, Ref. [15, Chapter 13]). Also, numerical calculations for some 'popular' potentials are indicative of an evident correlation between bound states and resonances.

With all due credit to modern numerical methods in quantum mechanics, it is worth emphasizing that more often than not they are based on the perturbation theory. This is also true, of course, of calculations in the Born approximation.

Under the assumption of small scattering phases δ_l ($l \neq 0$), the Pais approximation goes over into the Born approximation. On the other hand, the Pais approximation can also yield (at least in some cases) quasiclassical results. This is to a large extent due to the extension of the class of functions for which variational problems are formulated and solved. It is precisely such a program that produced new results on changing from half-integer order Bessel functions standardly used in quantum mechanics to arbitrary order Bessel functions. Clearly, other possible extensions of the class of variation functions are also of interest.

The problem of calculating scattering phases for particles with nonzero moments and arbitrary energies and potentials cannot, of course, be solved in the general case by numerical methods alone, and qualitative, analytical, and semi-analytical methods remain, of course, relevant and useful. While only a relatively few examples have been considered above, the very methods with which they were treated give rise to the hope of considerably extending the range of problems that are encountered in atomic, nuclear, and molecular physics and which can be approached using Pais type approximations.

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