NONRELATIVISTIC QUANTUM THEORY OF PARTICLE SCATTERING

V. D. Kamenetskii

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A method previously described [1-4] is further developed for radial equations for nonrelativistic quantum-mechanical problems on collisions.

This method [1-4] usually involves a fairly large volume of calculation, but it can be modified from [2, 3] for scattering in a central static field to reduce the volume considerably; the oscillatory part most slowly convergent at large r is first isolated in explicit form from the wave function for the scattered particle, which greatly eases the summation of the power series in [2], because these then converge much more rapidly. The symbols are as in [1-3].

The solution to a second-order radial equation

$$f_l''(r) + [\kappa^2 - r^{-2}(l+1)\,l - V(r)]\,f_l(r) = 0 \tag{1}$$

is sought in the form of two particular solutions

$$f_l(r) = A_l\,[f_l^+(r) + f_l^-(r)], \tag{2}$$

with

$$f_l^\pm(r) = a_l^\pm\,\varphi_l^\pm(r)\ \exp \pm i\kappa r, \tag{3}$$

the $a^\pm$ being arbitrary constants and the A_l normalization constants; $f_l(r)$ satisfies the boundary conditions

$$f_l(0) = 0; \tag{4}$$

$$f_l(r) \backsim \sin\left(\kappa r - \frac{l\pi}{2} + \eta_l\right). \tag{5}$$

We substitute (3) into (1) to get $\varphi_l^\pm(r)$ as

$$\varphi_l^{\pm\,''} \pm 2\,i\kappa\varphi_l^{\pm\,'} - [r^{-2}(l+1)\,l + V(r)]\ \varphi_l^\pm = 0. \tag{6}$$

It is readily shown that the regular functions φ^+ and φ^- are merely complex-conjugate functions; a^- also equals $(a^+)^*$, so we merely have to find $a_l^+\varphi_l^+(r)$ in order to solve the problem, in accordance with (2) and (3).

By analogy with (2), we seek a solution for $\varphi_l^+(r)$ around the first special point $r_0 = 0$ of (1) in the form

$$a_l^+\ \varphi_l^+(r) = a_l^+\sum_{n=l+1}^{\infty} C_{ln}^+ r^n = D_l^+\sum_{n=l+1}^{\infty}\alpha_{ln}^+ r^n = D_l^+ R_l^+(r). \tag{7}$$

As for (2), we have for α^+ the recurrence relation

$$\alpha_{ln}^+ = \frac{\sum\limits_{j=1}^{n-l-1}{}'' \, b_{j-2}\,\alpha_{l\,n-j}^+}{(n+l)\,(n-l-1)}, \tag{8}$$

$$\alpha_{l\,l+1}^+ = 1;\ n = l+2,\ l+3\ldots,$$

which gives any of the α_{ln}^+. The primes indicate that b_{-1} must be replaced by $b_{-1} - 2ik(n + l - 1)$ in the summation, in which the b_j are the coefficients in the V(r) of (2). The next special point of (1) lies at ∞, so (7) converges to the exact solution, in accordance with the general theory [5], at least for any finite r. This is sufficient to solve a collision problem, i. e., to determine the scattering phases.

A difference from [3] is that now (2), (3), and (5)-(7) show that $\overline{R}_l^+(r)$ for r large [but for the region in which (7) converges] tends to a finite value $\overline{R}_l^+$, which can be found from (8). The scattering phases have then to be expressed in terms of $\overline{R}_l^+$. The results of [1] may be utilized if we normalize the wave function as in [1] for the general case. It is convenient to represent the asymptote of the wave function of [1] as a sine wave of altered phase; then

$$\frac{1}{\kappa}\exp i\eta_l \sin\left(\kappa r-\frac{l\pi}{2}+\eta_l\right)=A_l\,(D_l^+\bar{R}_l^+\exp i\kappa r+D_l^-\bar{R}_l^-\exp-i\kappa r). \tag{9}$$

We use Euler's formula, equate coefficients to sin kr and cos kr, and use the fact that the minus signs in D^- and $\bar{R}^-$ are equivalent to the complex conjugates D^+ and $\bar{R}^+$ to get

$$\exp i\eta_l \cos\left(\eta_l-\frac{l\pi}{2}\right)=\kappa A_l i\,(D_l^+\bar{R}_l^+-D_l^{+*}\bar{R}_l^{+*}), \tag{10}$$

$$\exp i\eta_l \sin\left(\eta_l-\frac{l\pi}{2}\right)=\kappa A_l\,(D_l^+\bar{R}_l^++D_l^{+*}\bar{R}_l^{+*}). \tag{11}$$

We use the relation [1] between the asymptotic behavior and that at zero to get in the phase representation

$$\frac{i}{2}\,(1-\exp 2i\eta_l)=D_{ll}D_l\,|D_l|^{-2}. \tag{12}$$

But (2), (3), (7), and (8) imply that

$$D_l=A_l\,(D_l^++D_l^{+*}). \tag{13}$$

The last four equations contain only η_l, D_l^+, D_l, and A_l as unknowns, so we can express the scattering phases via these in terms of $\bar{R}_l^+$, which serves to solve the problem.

It is often convenient to take the arbitrary constants of (3) in the following form:

$$a_l^{\pm}=1/2A_lC_l^{\pm}. \tag{14}$$

This choice of the $a^{\pm}$ gives real wave functions, which are very convenient in numerical calculations. It has been shown [2] that the wave function in the general case can always be expressed as the product of a complex constant and a real function; the explicit form of this constant is extremely important in some theoretical studies [1] (since the scattering phase may be expressed in terms of it), but it does not need to be calculated in some cases, as in the computation of relative wave functions, which can [3] be used to find even the scattering phase if they are known for any r). In (14) $D_l^{\pm}=1/2A_l$.

The constants are thus chosen from (14); (11) is divided by (10) to give the scattering phases simply as

$$\mathrm{tg}\left(\eta_l-\frac{l\pi}{2}\right)=-\bar{R}_{lR}^+/\bar{R}_{lI}^+. \tag{15}$$

We must make r sufficiently large in the calculation of $\bar{R}_l^+$; see [3] for some estimates of how large r should be for electron-atom collisions. As in [3], the phase will not depend on the choice of r for r large.

This method has no advantages over those of [2, 3] for r small, as numerical calculations for electron scattering by hydrogen atoms have shown.

The modified method of [2] (insertion of an explicit oscillatory asymptote in the wave function for the scattered particle) can be used with particular solutions other than of the form of (3); solutions can be sought with the exponentials of (3) replaced by sin kr and cos kr, but then (6) is replaced by a differential equation in which the coefficient to $\varphi^{\pm'}$ is replaced by a function of r (either −2k tan kr or +2k cot kr). This gives a recurrence relation much more complex than (8), although the α are then real. There is also the difficulty that the poles are infinite in number, which demands a special examination of these. It can be shown from (3) and (7) that here $\varphi_l^+=R_{lR}^+$ and $\varphi_l^-=-R_{lI}^+$, and then the right side of (9) shows that (14) gives exactly the same result for the phases as do the functions of (3), but via much larger volumes of calculation.

There is exceptional interest (especially from the theoretical point of view) in the case $k\to 0$, because in this case (at least) there is no special point at ∞, so a power-series solution constructed near zero may be correctly extended to any infinitely remote point. The modified method is precisely that of [1-3] if k = 0, so the proof given below is applicable to both methods.

We examine the behavior at infinity by performing the usual $r = 1/z$ transform and examining $F(r) = f(r)/r$ for $z \to 0$. We have

$$F''(z) - z^{-4}V(z)F(z) = 0. \tag{16}$$

Consider electron-atom collisions; here for $z \to 0$

$$z^{-4}V(z) \sim z^{-4} \exp - \gamma^2/z \to 0,$$

because the exponential tends to zero more rapidly than any finite power of z; so $F''(z) = 0$ for $z \to 0$, and the equation has thus no special point at $z = 0$. Hence $F''(r) = 0$ for $r \to \infty$ has no special point either.

The oscillatory asymptote can also be used to modify the method [4] of solving problems on atomic excitation by electron impact.

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