

Numerical calculation of the S-state energy eigenvalues for a local potential

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gives surprisingly large reflections of the beam, because the disk becomes prismatic in section; fortunately, these deflections occur in a radial direction and can therefore be distinguished from the aberration effect, which is tangential. Moreover, they are independent of the sense of rotation, as are also any effects due to photoelastic polarization by the medium under centrifugal forces.

Figure 1 shows a record of the lateral position of the emergent light beam during a run with the disk rotational speed varying from 0 to +1800 to 0 to -1800 rpm. The broadening effect at low speeds is due to causes (i) to (iii) above; in addition the effect of a slight change of axis is apparent, also some zero drift; but, despite these defects, a general displacement proportional to and in the same sense as the transverse velocity of the disk is present. It can be seen on every run designed to detect a tangential displacement despite intentional changes in items such as the bearings. As for magnitude, with a glass disk of 19.1 mm thickness and refractive index 1.51 with white light passing twice through the disk at 110 mm radius from the axis of rotation, the displacement when the speed is increased from 600 to 1800 rpm should be about 1.49×10^{-6} mm from Fresnel's formula; the preliminary experiment gives 1.50×10^{-6} mm $\pm 10\%$.

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Numerical calculation of the S-state energy eigenvalues for a local potential

Abstract. A numerical method for calculating the S-state energy eigenvalues for a local potential is given. The method makes use of a first-order differential equation which is easily derived from the Schrödinger equation.

One of the important problems in quantum mechanics is the calculation of the energy eigenvalues for a particular potential in the Schrödinger equation, that is, given the potential V between two particles we wish to solve the equation

$$(T + V)\Psi = E\Psi \quad (1)$$

where T is the kinetic energy, for the negative energy (or energies), $E = -E_B$. For most potentials an algebraic solution of equation (1) cannot be found and numerical methods have to be used. In this letter, a simple method to calculate the S-state

L4 Letters to the Editor

energy eigenvalues is outlined. This method is ideally suited for the electronic computer. In addition, the method can be used to determine the total number of bound S-states for a given potential, provided that this number is finite.

The Schrödinger equation for the S-state and negative energies is

$$\frac{d^2u(r)}{dr^2} - V(r)u(r) = \mu^2u(r)$$

$$u(0) = 0 \quad (2)$$

where the potential $V(r)$ is measured in units $(\text{length})^{-2}$ and the binding energy ($\mu = \mu_B$) is $\hbar^2\mu_B^2/2m$, m being the reduced mass. Beyond the range R of the potential the solution of equation (2) for $\mu = \mu_B$ has the form

$$u_B(r) \underset{r \gg R}{\simeq} e^{-\mu_B r}.$$

The logarithmic derivative of the wavefunction $u(r)$ is $y(r) = u^{-1} du/dr$. It is a simple matter to show that it satisfies the differential equation

$$\frac{dy}{dr} = \mu^2 - y^2 + V(r). \quad (3)$$

The boundary condition for the integration of equation (3), the Riccati equation, is $y(0) = \infty$. At the energy of a bound state, $y(\infty) = -\mu_B$. On account of the boundary condition, the numerical integration of equation (3) is impractical. However, using the transformation

$$y(r) = \mu \cot f_\mu(r) \quad (4)$$

we find that the function $f_\mu(r)$ satisfies the differential equation

$$\frac{df_\mu}{dr} = -\frac{V(r)}{2\mu}(1 - \cos 2f_\mu) + \mu \cos 2f_\mu \quad (5)$$

with the boundary condition $f_\mu(0) = 0$. At an energy of a bound state

$$f_\mu(r) \underset{r \gg R}{=} (n + \frac{3}{4})\pi. \quad (6)$$

We note that the transformation (4) is very similar to the one used for positive energies (i.e. $y(r) = k \cot(\delta(r) + kr)$, where $\delta(\infty)$ is the phase shift) to obtain the phase equation (Calogero 1967, Kermode and Sprung 1969).

The solution of equation (2) for arbitrary μ has the asymptotic form

$$u(r) \underset{r \gg R}{\simeq} a(\mu) e^{\mu r} + b(\mu) e^{-\mu r} \quad (7)$$

where $a(\mu)$ and $b(\mu)$ are related to the potential $V(r)$, so that

$$f_\mu(r) \underset{r \gg R}{\simeq} \arctan \left(\frac{a(\mu) e^{2\mu r} + b(\mu)}{a(\mu) e^{2\mu r} - b(\mu)} \right). \quad (8)$$

If $\mu r \gg 1$ and $\mu \neq \mu_B$, then

$$f_\mu(r) \underset{r \gg R, \mu r \gg 1}{\simeq} \arctan(1) = (n + \frac{1}{2})\pi. \tag{9}$$

For zero energy, the asymptotic form of the wavefunction is

$$u(r) \simeq a_0 r + b_0.$$

Hence,

$$f_0(r) \underset{r \gg R, \mu \rightarrow 0}{\simeq} \lim \arctan\{\mu a_0^{-1}(a_0 r + b_0)\} = \begin{cases} n\pi & \text{if } a_0 \neq 0 \\ (n + \frac{1}{2})\pi & \text{if } a_0 = 0. \end{cases} \tag{10}$$

The case $a_0 = 0$ corresponds to a bound state at zero energy. Equations (5), (6), (9) and (10) are very useful for the determination of a binding energy and we now illustrate the method with the application to the Yukawa potential

$$V(r) = -1.5186 \frac{e^{-0.34r}}{r} \text{ fm}^{-2}. \tag{11}$$

(There is nothing extraordinary about this particular potential; it arose from a study of potentials having a small scattering length.) The differential equation (5) was integrated out to 20 fm for various values of μ . It was found that $f_\mu(20) = g(\mu)$ is a continuous function of μ (the solution of equation (3) is not) with, for example, $g(\epsilon) = \pi$ (for ϵ very small), $g(0.1) = 3.928 (\simeq \frac{5}{4}\pi)$ and $g(0.2) = 0.7859 (\simeq \frac{1}{4}\pi)$. Immediately, we have that $0.1 < \mu_B < 0.2$. Further calculations gave $g(0.19981) = 3.897$ and $g(0.19982) = 0.7941$ and eventually $\mu_B = 0.1998122$. In view of the large number of decimal places, the step length was halved from 0.01 to 0.005. The result was not affected.

Next, the depth of the potential (10) was increased. It was found that, in the limit, $g(0) = n\pi$, where n is the number of bound states (apart from the case of a bound state at zero energy). This is related to Levinson's theorem. It was also found that $g(\mu) \simeq (n + \frac{1}{2})\pi$ for μ small but greater than 0.05 and $g(\mu_B) \simeq (n + \frac{3}{2})\pi$ at the n th excited state.

Hence, this method gives a fast and accurate numerical calculation of the number and values of the S-state energy eigenvalues for a given local potential. The extension of the method to higher angular momentum states is at present being considered.

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