Theoretical physics made easy

Kyle Forinash
Natural Science Department, Indiana University—Southeast, New Albany, Indiana 47150

Jeff Irick[a]
Physics Department, East Tennessee State University, Johnson City, Tennessee 37614

(Received 14 June 1987; accepted 8 September 1987)

Advanced undergraduate physics students may benefit from theoretical computational tasks that involve relatively low study time. An example from nuclear physics is given in which packaged subroutines allow efficient computation of a nucleon interaction potential.

INTRODUCTION

Because theoretical physics often relies heavily on numerical techniques, it is sometimes difficult to find research projects that are mathematically simple enough for undergraduate students to complete in a semester or even an entire year. Most students have not had enough training in mathematics or numerical methods to do realistic theoretical problems, and assigning simplified problems may leave the student with the impression that theoretical problems always have convenient closed-form solutions. The use of prewritten subroutines is an effective way to circumvent this problem. While students should always be encouraged to learn to write their own computer programs, a senior research project is an excellent place to introduce some of the numerical shortcuts used by real engineers and physicists.

I. EXAMPLE

As an example of a realistic problem that can be reduced in complexity by using prewritten subroutines, consider plotting the following nuclear potential as a function of radius r:

$$V(r) = \left(\frac{g}{2M}\right)^2 \times \sum_{n=0}^{\infty} \frac{\Gamma(2qn+2)(2qn+1)^{2qn-2}(\zeta_q)^{2n}[C_n^{1/2q}(\xi_q)]^2}{\Gamma(qn+1)2^{qn}(m_{qn})^{2qn-3}} \times \frac{1}{6\sqrt{2}\pi^{3/2}}\,[2x_{qn}^{qn-1/2}K_{qn-5/2}(x_{qn}) - 3x_{qn}^{qn-3/2}K_{qn-3/2}(x_{qn})],$$

where

$$x_{qn} = (2qn+1)mr, \quad \xi_q = 1/4\zeta_q(q+1)m^2,$$

$$\zeta_q = \left(\frac{\lambda_1^2}{16(q+1)^2m^4} - \frac{\lambda_2}{4(2q+1)m^2}\right).$$

Here M is the nucleon mass, m is the pion mass, g is the nucleon–pion coupling constant, $\Gamma(qn+1)$ is the gamma function, $C_n^{1/2q}(\xi_q)$ is a Gegenbauer polynomial of order $1/2q$, and $K_{qn-3/2}(x_{qn})$ is a modified Bessel function of the second kind of fractional order. The values λ_1 and λ_2 are empirically derived nucleon–nucleon coupling constants, and $2q$ is the power of the interaction term in the field equation from which the potential was derived.

This potential has been shown[1] for choices of $n = 1$, $q = 1$, and $\lambda_2 = 0$ to match soft-core nuclear potentials constructed from nucleon scattering data.[2] Here we see that real life potentials are rather more formidable than simple potential models such as the Yukawa potential.

Writing a program to evaluate this potential is difficult for students because subroutines to evaluate gamma functions, Gegenbauer polynomials, and modified Bessel functions must be included. To avoid some of these technical difficulties and get to the physics in the problem it is convenient to use prewritten subroutines available on many mainframe computers.

II. METHOD

Figure 1 is a sample FORTRAN program that uses a subroutine from the mathematical and statistical package called IMSL (International Mathematical and Statistical Libraries) to evaluate the modified Bessel function of the second kind of fractional order. Job control statements (not shown) alert the computer that a special library should be searched for subroutines. The subroutine that evaluates the Bessel function is activated by the one-line FORTRAN statement CALL MMBSKR(ARG,ORDER,N,BK,IER). Here ARG is the argument of the Bessel function to be evaluated; ORDER is the order of Bessel function desired. The subroutine automatically calculates higher orders up to order ORDER + N in integer steps, where BK(N) is the output array multiplied by exp(ARG) and IER is an output error parameter. An IER of zero indicates successful evaluation of the Bessel function, an IER of 129 means an incorrect range of parameters ARG,ORDER or N, and an IER of 130 is returned if the subroutine encounters a value larger than machine infinity.

Figure 2 shows three plots of the potential for three sets of the values λ_1 and λ_2 with $q = \frac{3}{2}$ and the infinite series truncated at $n = 5$. The IMSL subroutines were used by a student to evaluate the gamma and Bessel functions, the Gegenbauer polynomials, and to calculate the poten-

[a] Now a graduate student in the physics department at Clemson University, Clemson, South Carolina.

input:

```
INTEGER N,IER
REAL ARG,ORDER
REAL*8 BK(5),BESS(5)
ARG=2.
ORDER=0.5
N=5
D=ORDER
CALL MMBSKR(ARG,ORDER,N,BK,IER)
   DO 30 J=1,5
     BESS(J)=BK(J)/EXP(ARG)
     WRITE(6,10)D,BESS(J),IER
     D=D+1.
30 CONTINUE
10 FORMAT (' ','BESSEL FUNCTION OF ORDER',I2,' IS ',
  ?E20.10,2X,' IER= ',I3)
   STOP
   END
```

output:

```
BESSEL FUNCTION OF ORDER 0.5 IS 0.1199377716D+00   IER= 0
BESSEL FUNCTION OF ORDER 1.5 IS 0.1799066611D+00   IER= 0
BESSEL FUNCTION OF ORDER 2.5 IS 0.3897977729D+00   IER= 0
BESSEL FUNCTION OF ORDER 3.5 IS 0.1154401114D+01   IER= 0
BESSEL FUNCTION OF ORDER 4.5 IS 0.4430201735D+01   IER= 0
```

FIG. 1. Example program using the IMSL subroutine MMBSKR.

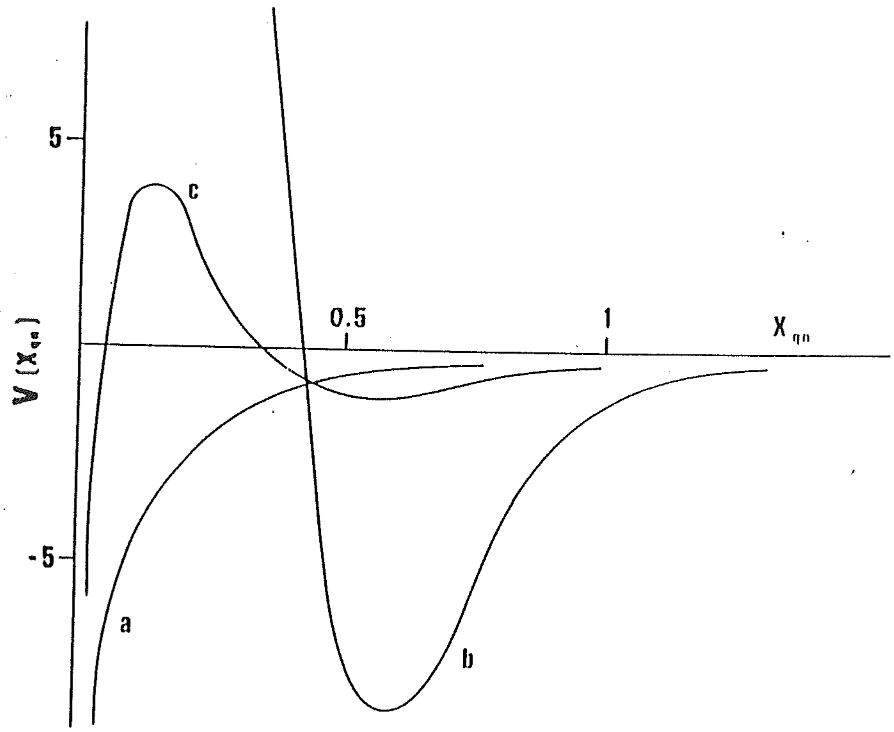

FIG. 2. The nuclear potential $V(x_{qn})$ in MeV plotted as a function of $x_{qn} = (2qn + 1)\, mr$ where r is the radial distance.

tial for these plots. The shape shown in curve c is previously unreported for this potential.

Just as anyone using a hand calculator should be aware of its limits of accuracy (for example, round-off error), students should understand the subroutine they are using even if they did not write it. For example, the MSL package provides documentation for all the subroutines in its library, explaining the technique used including references to relevant literature. The subroutine MMBSKR is based on Temme's algorithm and work done by J. B. Campbell.[3] Information about Bessel functions and other special functions can be found in many standard references.[4]

III. CONCLUSIONS

Certainly students in a numerical methods class should be required to learn standard techniques for problems such as evaluating integrals and solving differential equations. However, there is no point in duplicating the work of others when doing a numerical calculation in theoretical physics. Prewritten subroutines can be an effective tool for students of theoretical physics to learn about special functions and see good examples of numerical methods without getting bogged down in the details of numerical techniques.

REFERENCES

1. M. Sebhatu, Lett. Nuovo Cimento **36**, 513 (1983).
2. R. V. Reid, Ann. Phys. **50**, 411 (1968).
3. IMSL Library Contents Document (1984).
4. *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (National Bureau of Standards, Washington, DC, 1972).