Using the NAG Library for quantum dot computations.

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A second-year (post)graduate student from Africa visiting ICTP needed some help with his numerical computation involving quantum dots.

The Hamiltonian for the quantum dot was described in the single-electron approximation. He was using the variational approach to Schrödinger's equation in order to obtain the ground state energy of a quantum dot having a single-site impurity. The effect of the application of an electric field also needed to be considered.

The integrals, most of them two-dimensional (2D), needed to solve the problem are obtained numerically. One of his goals was to obtain the ground state energies for varying electric-field strengths. In addition to the energies, he also wanted to obtain the polarizabilities when different electric fields are applied to the system - this involves yet another (smaller) set of integrals.

First, I tried to modify a one-dimensional integration routine from some other source to perform the required 2D integrals - by calling a function which calls another function, unfortunately, this proved to be ineffective. The NAG Library came to the rescue. I used one of NAG's 2D integration routines (d01daf) to compute the value of the required integrals.

I. PROBLEM

The system is a quantum dot with a charge impurity placed in an electric field. The Hamiltonian in Rydberg atomic units is:

$$H = -\nabla^2 - \frac{2}{\boldsymbol{r} - \boldsymbol{r}_0} + f(r\cos\theta - r_0) + V(r). \tag{1}$$

Here, $\boldsymbol{r}$ is the position of the electron, $\boldsymbol{r}_0$ is the (fixed) position of the impurity, $V(r)$ is the confining potential for the electron, $r = |\boldsymbol{r}|$ and $r_0 = |\boldsymbol{r}_0|$. The angle θ is that between the electric field vector and $\boldsymbol{r}$ with f being the strength of the field.

To find the ground state energy of the system, One can assume a trial wavefunction $\psi(\boldsymbol{r};\alpha,\beta,f)$ with parameters α and β and then minimize the trial energy E_T with respect to these parameters. The trial energy E_T is given by:

$$E_T = \frac{\int \psi^*(\boldsymbol{r};\alpha,\beta,f) H \psi(\boldsymbol{r};\alpha,\beta,f) d^3r}{\int \psi^*(\boldsymbol{r};\alpha,\beta,f)\psi(\boldsymbol{r};\alpha,\beta,f) d^3r} \tag{2}$$

Invariably, the integrals above end up being sums of 2D integrals a couple of which are:

$$\begin{aligned} I_4 = & \int_a^b \int_0^\pi \frac{\sin^2[K(r-a)]}{r} \frac{[2*(r^2+r_0^2) - rr_0(1+3\cos^2\theta)]\cos\theta}{(r_0^2+r^2-2rr_0\cos\theta)^{3/2}} \\ & \times \exp(-2\alpha\sqrt{r_0^2+r^2-2rr_0\cos\theta}) d\theta dr \end{aligned} \tag{3}$$

and

$$\begin{aligned} M_3 = & \int_a^b \int_0^\pi (r\cos\theta - r_0)^2 \sin\theta \sin[K(r-a)] \cos[K(r-a)] \frac{[r - r_0\cos\theta]}{\sqrt{r_0^2+r^2-2rr_0\cos\theta}} \\ & \times \exp(-2\alpha\sqrt{r_0^2+r^2-2rr_0\cos\theta}) d\theta dr \end{aligned} \tag{4}$$

Here, $K = \pi/(b-a)$ and a and b are the inner and outer radii, respectively, of the circular quantum dot. I used the routine `d01daf` from the NAG Library to successfully compute these 2D integrals conveniently and easily.

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