The Abdus Salam International Centre for Theoretical Physics

利用 NAG 算法库计算量子点

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国际理论物理中心来自非洲的博士后研究员，需要数值计算协助，从事量子点 (quantum dot) 的计算。

量子点的 Hamiltonian 是在单电子近似中被描述。为了要在有单部位杂质的量子点中取得原始的能量，他于是在薛丁格方程式 (Schrödinger's equation) 中使用 variational 方法。同时，电子场的应用效果也必须考虑 。

式子中大部分都是二重积分，必须以数值方法求解。他的目的之一，就是要在各种不同电子场的强度中取得原始能量。除了能量外，他同时也想要了解在系统中使用不同电场的极化率 (polarizabilities) – 这当然也涉及到较小的积分问题。

首先，我想要修改从其他来源拿到的一阶积分函数，透过函数来调用另一函数来解决我的二重积分问题。然而，最后我意识到这样做效率极低。NAG 算法库解救了我。我使用 NAG 算法库中的二重积分函数 (d01daf)，计算我所要求解的积分问题。

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:

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

and

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

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.