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The Numerical Solution of Schrödinger's Equation with a Nonlocal Potential*

In a recent paper [1], we suggested a new method for the numerical solution of Schrödinger's equation, based on the following approximation for two non-commuting operators H_0 and H_1,

$$e^{-\beta(H_0+H_1)} = e^{-1/2\beta H_1} e^{-\beta H_0} e^{-1/2\beta H_1} + 0(\beta^3). \tag{1}$$

Moreover, the error in making this replacement can be found from the evaluation of the expectation value of the next term, viz.,

$$\tfrac{1}{12}\beta^3 e^{-1/2\beta H_1} e^{-1/2\beta H_0}\{\tfrac{1}{2}[H_1, (H_1, H_0)] + [H_0, (H_1, H_0)]\} e^{-1/2\beta H_0} e^{-1/2\beta H_1}.$$

We would like to point out that this method also provides for a simple numerical solution of Schrödinger's equation with a nonlocal potential.

For such a case, we consider the equation

$$-\frac{\partial^2}{\partial \mathbf{x}^2}\Psi(\mathbf{x}, \beta) + \int d\mathbf{x}'\, V(\mathbf{x}, \mathbf{x}')\, \Psi(\mathbf{x}', \beta) = -\frac{\partial \Psi}{\partial \beta}(\mathbf{x}, \beta), \tag{2}$$

where $V(\mathbf{x}, \mathbf{x}')$ is a nonlocal potential, and β is a real parameter. To solve this equation, we use the same approach as [1], repeating the basic steps here, in a slightly modified form, to make this note self-contained. By separating Eq. (2) into spherical polar coordinates (r, θ, ϕ), and expanding in spherical harmonics, we may rewrite this as

$$\begin{aligned} -\left(\frac{\partial \phi_l}{\partial \beta}\right) &= H_0\phi_l + H_1\phi_l \\ &= \left[-\frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{r^2}\right] \phi_l(r, \beta) + \int_0^\infty v_l(r, r')\, \phi_l(r', \beta)\, dr', \end{aligned} \tag{3}$$

where $\phi_l(r, \beta) = r\psi_l(r, \beta)$ (i.e., $\phi_l(0, \beta) = 0$) and $v_l(r, r')$ is defined via

$$V(\mathbf{x}, \mathbf{x}') = \sum_{l=0}^{\infty} \frac{(2l+1)}{4\pi r r'} v_l(r, r')\, P_l(\cos \alpha),$$

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where $\cos\alpha = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi - \phi')$. The solution of this equation can be written formally as

$$\phi_l(r, \beta) = e^{-\beta(H_0+H_1)}\,\phi_l(r, 0) \tag{4}$$

and, hence, using Eq. (1),

$$\phi_l(r, \beta) = e^{-1/2\beta H_1}\, e^{-\beta H_0}\, e^{-1/2\beta H_1}\phi_l(r, 0) + O(\beta^3) \tag{5}$$

gives the solution for sufficiently small β. Writing $\rho_l(r, r', \beta)$ and $G_l(r, r', \beta)$ for the configuration space representation of the operators $\exp(-\beta H_0)$ and $\exp(-\frac{1}{2}\beta H_1)$, this equation becomes

$$\phi_l(r, \beta) = \int_0^\infty dr' \int_0^\infty dr_1 \int_0^\infty dr_2\, G_l(r, r_1, \beta)\, \rho_l(r_1, r_2, \beta)\, G_l(r_2, r', \beta)\, \phi_l(r', 0). \tag{6}$$

Extracting the explicit β dependence, it is easily seen that the eigenvalues (E_n) and eigenfunctions $[\phi_n(r)]$ of the Schrödinger equation corresponding to Eq. (3) satisfy the integral equation,

$$e^{-\beta E_n}\phi_n(r) = \int_0^\infty dr' \int_0^\infty dr_1 \int_0^\infty dr_2\, G_l(r, r_1, \beta)\, \rho_l(r_1, r_2, \beta)\, G_l(r_2, r', \beta)\, \phi_n(r'). \tag{7}$$

For the appropriate boundary conditions, it is easy to find an expression for $\rho_l(r, r', \beta)$ in closed form,

$$\rho_l(r, r', \beta) = \frac{4\pi}{(4\pi\beta)^{3/2}}\, e^{-(r^2+r'^2)/4\beta} rr' i_l\left(\frac{rr'}{2\beta}\right), \tag{8}$$

where i_l is the modified spherical Bessel function. The function $G_l(r, r', \beta)$ can be written as an expansion in powers of β, thus,

$$G_l(r, r', \beta) = \delta(r - r') - \frac{1}{2}\beta v_l(r, r') + \frac{1}{8}\beta^2 \int_0^\infty v_l(r, r'')\, v_l(r'', r')\, dr'' + O(\beta^3). \tag{9}$$

Under these circumstances, Eq. (7) becomes a homogeneous integral equation with symmetric kernel, whose eigenvalues and eigenfunctions can be found by standard numerical techniques.

By cutting off the integrals in Eq. (7) at some finite point (R), and calculating them by quadratures, the problem becomes one of finding the eigenvalues and eigenvectors of the matrix equation,

$$e^{-\beta E}\phi_i = \sum_{j=1}^{N} A_{ij}\phi_j\,, \tag{10}$$

where

$$A_{ij} = \sum_{k,l=1}^{N} Q_{ij} P_{kl} Q_{lj} ,$$

$$Q_{ij} = \Delta G_l(r_i , r_j', \beta), \qquad P_{ij} = \Delta \rho_l(r_i , r_j', \beta),$$

$$\phi_i = \phi(r_i),$$

and

$$r_i = i\Delta, \qquad i = 1,..., N, \qquad \Delta = R/N,$$

with the proviso that β and Δ be small and $\Delta^2/4\beta \ll 1$. There is no essential difficulty associated with the δ function appearing in Eq. (9), since it always appears as an integrand. In our finite difference representation, this term contributes a factor 1 to the diagonal elements and zero to the off-diagonal elements of the matrix Q_{ij}.

As an example, we have considered a potential with a Gaussian nonlocality,

$$V(\mathbf{x}, \mathbf{x}') = \sqrt{u(r)\, u(r')}\, \frac{1}{(\pi\gamma^2)^{3/2}}\, e^{-(\mathbf{x}-\mathbf{x}')^2/\gamma^2}. \tag{11}$$

In this case, we have

$$v_l(r, r') = \sqrt{u(r)\, u(r')}\, \frac{rr'}{(\pi\gamma^2)^{3/2}}\, e^{-(r^2+r'^2)/\gamma^2}\, i_l\left(\frac{2rr'}{\gamma^2}\right). \tag{12}$$

We have performed the calculations for the eigenvalues of the $1S_{1/2}$, $2S_{1/2}$ and $1P_{3/2}$ levels in a shell model potential appropriate to the C_6^{12} nucleus [2]. For this case, we have a Wood-Saxon potential as the central part, $u(r)$, of our nonlocal potential,

$$u(r) = -\frac{V_0}{[1 + e^{(r-R)/\alpha}]}, \qquad R = r_0 A^{1/3},$$

with the parameters, $V_0 = 90$ MeV, $r_0 = 1.04$ F, $\alpha = 0.65$ F. The calculations also included a local spin-orbit coupling contribution

$$V^{\text{spin}}(r) = -\left(\frac{h}{m_\pi c}\right)^2 \frac{V_s}{V_0} \frac{1}{r} \frac{\partial u(r)}{\partial r}\, \underline{l} \cdot \underline{\sigma}, \tag{13}$$

with $V_s = 24.65$ MeV, and a local Coulomb potential due to a uniform sphere of equal charge to that of the nucleus. The results of these calculations, for various values of the nonlocality parameter γ, are shown in Fig. 1. This method has the advantage of being fast (10 sec for a 60 point grid for each value of γ on a CDC

6400) and stable and avoids the approximations introduced by either the effective mass approximation [2] or the local energy approximation ([3], [4]).

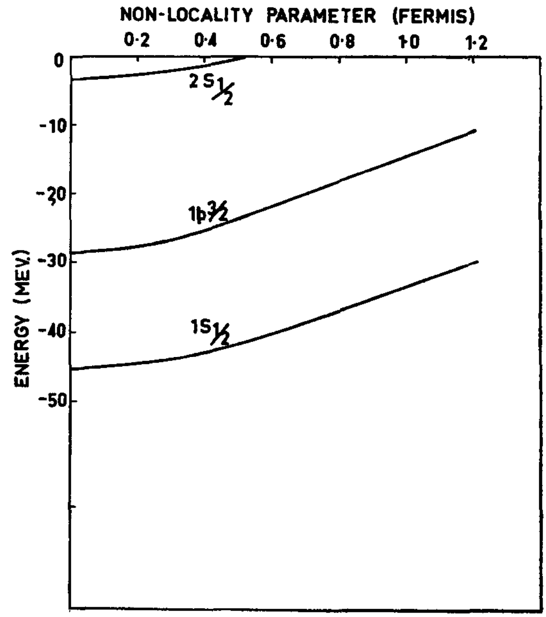

FIG. 1. Shell model calculations for the energy values of the $1S_{1/2}$, $2S_{1/2}$, $1P_{3/2}$ levels of the C_6^{12} nucleus as a function of the nonlocality parameter γ.

$R = 12.0$ F, $N = 60$, $\beta = 0.003$.

Finally, we should like to point out that, at least in principle, there is no real problem connected with the introduction of spin. The spin-orbit coupling potential, Eq. (13), does not couple the various spin states, and we have simply different potentials occuring for the two spin directions. In the most difficult situation, with tensor forces, there will be a mixing of different states, so that Eq. (7) must be replaced by a set of coupled integral equations. The numerical solution of this set will still be possible by a difference scheme leading to a system of equations analogous to Eq. (10). Of course, the dimension of the matrix A_{ij} (which is determined by the degree of intermixing of the various states) will eventually determine the feasibility of carrying out any numerical calculations.

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