RESEARCH NOTES

Approximation on computing partial sum of nonlinear differential eigenvalue problems*

SUN Jiachang (孙家昶)[1]** and JIANG Murong (蒋慕蓉)[1,2]

1. Institute of Software, Chinese Academy of Sciences, Beijing 100080, China;

2. Department of Mathematics, Yunnan University, Kunming 650091, China

Received January 9, 2001; Revised February 27, 2001

Abstract In computing the electronic structure and energy band in a system of multi-particles, quite a large number of problems are referred to the acquisition of obtaining the partial sum of densities and energies using the "first principle". In the conventional method, the so-called self-consistency approach is limited to a small scale because of high computing complexity. In this paper, the problem of computing the partial sum for a class of nonlinear differential eigenvalue equations is changed into the constrained functional minimization. By space decomposition and perturbation method, a secondary approximating formula for the minimal is provided. It is shown that this formula is more precise and its quantity of computation can be reduced significantly.

Keywords: nonlinear eigenvalue problems, approximating algorithm, perturbation.

Nonlinear differential eigenvalue problems are the basic ones in calculating the energy functions for multi-particles in physics, chemistry and materials science. There are two ways to carry out the approximate computations: one is to choose appropriate basic functions and the other is to improve effective potential functions. As the physical wave function near the atomic nucleus varies very fast with space coordinates, these algorithms would reach convergence slowly, or lead to big errors or lower precision. Especially in computing electronic structure and energy band in a system of multi-particles, a number of problems are to get the partial sum of the densities and energies using the "first principle". The ordinary so-called self-consistency approach needs to calculate all or most of the eigenvalues and eigenfunctions. As the atoms increase in number, the computation becomes more complicated and troublesome. In 1996, Sun[1] proposed a block eliminating iteration method for solving higher-order generalized eigen-problems using the self-consistency approach and parallel block Jacobi method, and considered a couple of complex conjugate symmetric matrixes with 1572 orders in nonlinear optical crystal electronic structure problems. In 1997, Bai[1)] discussed the computing of partial eigenvalue sum for linear problems. In this paper, we change the problem of computing the partial sum for a class of nonlinear differential eigenvalue equations into one of the constrained functional minimization. By space decomposition and perturbation method, a secondary approximating formula for the minimal

* Project supported by the Major Basic Project of China (Grant No. G19990328) and the National Natural Science Foundation of China (Grant No. 10001032).

** Email: sun@mail.rdcps.ac.cn

1) Bai, Z. et al. Computing partial eigenvalue sum in electronic calculation, Research Report, 1997.

is provided. The numerical experiments show that this formula is more precise and its quantity of computation can drop significantly.

The nonlinear differential eigenvalue problem for describing the motion of multi-particles in a bounded domain is given as

$$\begin{cases} Lu_k + V(x)u_k + \varepsilon f(\rho)u_k = \lambda_k u_k, & k = 1,2,\cdots,q, \\ u_k \mid_{\partial\Omega} = 0, \end{cases} \tag{1}$$

where L is a quadratic linear bounded operator satisfying $(Lu, v) = (v, Lu)$; u_k the real-value eigenfunction corresponding to the eigenvalue λ_k; $\rho = \sum_{k=1}^{q} u_k^2$ the density function; $(u_k, u_j) = \delta_{kj}$, $k, j = 1,2,\cdots,q$. $|f(\rho)| \leqslant C|\rho|^r$, $0 < r \leqslant 2$; C and r are constants; $V(x)$ is a given potential function; ε a parameter; Ω a bounded domain in $\mathbb{R}^n$.

By the theory of differential equation, we know that there exists a weak solution $u_k \in H_0^1(\Omega)$, $k = 1,2,\cdots,q$ such that $\boldsymbol{u} = (u_1, \cdots, u_q) \in (H_0^1(\Omega))^q = H_0^1(\Omega) \times \cdots \times H_0^1(\Omega)$.

1 Ordinary algorithm

In dealing with electron states and relational physical properties for a system composed of a large amount of particles, most computing methods based on Kohn-Sham scheme, such as pseudopotential, linearized muffin-tin orbital method and linearized augmented-plane-wave method, have the following solving procedures.

(i) Choose a group of basic functions ϕ_r, $r = 1,\cdots,N$, $N > q$ to find an initial function $u_k^0 = \sum_{r=1}^{N} c_{kr}\phi_r$ with $(u_k^0, u_j^0) = \delta_{kj}, (k, j = 1,2,\cdots,q)$, and to obtain the initial density function value $\rho_0 = \sum_{k=1}^{q} (u_k^0(x))^2$;

(ii) solve the iterated equations $Lu_k^m + V(x)u_k^m + \varepsilon f(\rho^{m-1})u_k^m = \lambda_k^m u_k^m$ to get u_k^*, $\lambda_k^* (k = 1,2,\cdots,q)$, and $\rho^m = \sum_{k=1}^{q} (u_k^m(x))^2$;

(iii) if $\| \rho^m - \rho^{m-1} \|$ is less than the number given first, then stop; otherwise replace the initial density function, iterate again;

(iv) sort λ_k from small to large, count the sum of q eigenvalues $\tilde{\mu}_q = \sum_{k=1}^{q} \lambda_k$.

Usually, the number of atoms N is 10 ~ 100 times of q. If N is 100, the order of matrix needed to be computed will be $10^4 \sim 10^5$, and if N is 1000, the matrix order will reach 10000 ~ 100000. The computing process becomes more and more complicated and difficult.

2 Approximating formula

Define a functional[1)]

1) Sun, J.C. Density functional approach for computing partial eigenvalue sum instead of self-consistency approach. 1999 RDCPS Annual Reports, 1 ~ 4.

$$I(\boldsymbol{u}) = \sum_{k=1}^{q}(Lu_k + V(x)u_k,\ u_k) + \varepsilon\int_{\Omega} f(\rho)\rho \mathrm{d}\Omega, \tag{2}$$

where $\boldsymbol{u} = (u_1,\ u_2,\ \cdots,\ u_q)$, $u_k \in H_0^1(\Omega)$, $(u_k, u_j) = \delta_{kj}$, $(k, j = 1,2,\cdots,q)$, $\rho = \sum_{k=1}^{q} u_k^2$.

As $I(\boldsymbol{u})$ is the expected value of total energy for a given q particle system, we call $I(\boldsymbol{u})$ the energy functional.

From (2), it is easy to know that the functional $I(\boldsymbol{u}) \in (H_0^1(\Omega))^q$ is (i) well defined; (ii) lower semibounded; (iii) coercive; (iv) lower semicontinued. By Theory 1.2 in Ref. [2], the functional $I(\boldsymbol{u})$ can attain its infimum in $(H_0^1(\Omega))^q$. It is not difficult to prove that[3] this minimization is a weak solution of problem (1).

In order to get partial eigenvalue sum for problem (1), one needs to compute

$$\mu_q = \min I(\boldsymbol{u}). \tag{3}$$

If $\varepsilon = 0$, problem (1) becomes q independent linear equations $\bar{L}u = Lu + V(x)u = \lambda u$, each of which is solvable and has a unique minimum. They may form an orthogonal matrix. By orthogonal transformation, we can change this orthogonal matrix into a diagonal matrix, then take the diagonal functions as the initial values, then use the perturbation method to approximate (3).

For simplicity, we denote the diagonal functions by u_{k0}, $k = 1,2,\cdots,q$.

When $\varepsilon \neq 0$, we decompose $H_0^1(\Omega)$ into $H_0^1(\Omega) = H_{0q}^1(\Omega) \oplus (H_{0q}^1(\Omega))^{\perp}$, where

$$H_{0q}^1 = \mathrm{Span}\{u_{k0} \mid \bar{L}u_{k0} = \lambda_{k0}u_{k0},\ (u_{k0},\ u_{j0}) = \delta_{kj},\ k,\ j = 1,\cdots,q\}.$$

Then, for $u_k \in H_0^1(\Omega)$, one has

$$u_k = p_k u_{k0} + \varepsilon g_k u_{k1}, \quad u_{k0} \in H_{0q}^1(\Omega), \quad u_{k1} \in (H_{0q}^1(\Omega))^{\perp}. \tag{4}$$

If $u_k (k = 1,2,\cdots,q)$ is a solution of problem (1), by the orthogonality of u_k, one obtains

$$\varepsilon^2 g_k g_j (u_{k1},\ u_{j1}) = \begin{cases} 0, & k = j, \\ 1 - p_k^2, & k = j. \end{cases} \tag{5}$$

if $g_k \neq 0$, then $p_k^2 + (\varepsilon g_k)^2 = 1$. Substituting (4) into (2), with (5), we have

$$\begin{aligned} I(\boldsymbol{u}) &= I(\boldsymbol{u}_0) \\ &+ \varepsilon^2 \sum_{k=1}^{q} [(\bar{L}u_{k1},\ u_{k1}) - (\bar{L}u_{k0},\ u_{k0})] \left[g_k + \frac{((f(\rho_0) + \rho_0 f'(\rho_0))u_{k0},\ u_{k1})}{(\bar{L}u_{k1},\ u_{k1}) - (\bar{L}u_{k0},\ u_{k0})} p_k \right]^2 \\ &- \varepsilon^2 \sum_{k=1}^{q} \frac{((f(\rho_0) + \rho_0 f'(\rho_0))u_{k0},\ u_{k1})^2}{(\bar{L}u_{k1},\ u_{k1}) - (\bar{L}u_{k0},\ u_{k0})} p_k^2 + O(\varepsilon^3 g_k^2), \end{aligned} \tag{6}$$

$$\rho_0 = \sum_{k=1}^{q} (u_{k0})^2, \quad I(\boldsymbol{u}_0) = \sum_{k=1}^{q} [(\bar{L}u_{k0}, u_{k0}) + \varepsilon(f(\rho_0)u_{k0}, u_{k0})]. \tag{7}$$

If $(\bar{L}u_{k1}, u_{k1}) - (\bar{L}u_{k0}, u_{k0}) < 0$, let $g_k = 0$; otherwise

$$g_k = -\frac{((f(\rho_0) + \rho_0 f'(\rho_0))u_{k0}, u_{k1})}{(\bar{L}u_{k1}, u_{k1}) - (\bar{L}u_{k0}, u_{k0})} p_k. \tag{8}$$

Then $I(\boldsymbol{u}) = I(\boldsymbol{u}_0) - \varepsilon^2 \sum_{k=1}^{q} [(\bar{L}u_{k1}, u_{k1}) - (\bar{L}u_{k0}, u_{k0})] g_k^2 + O(\varepsilon^3 g_k^2)$.

Now, problem (3) has changed into a problem of how to select u_{k1} and g_k such that

(i) $\varepsilon^3 g_k^2 < 1$;

(ii) $w_k = [(\bar{L}u_{k1}, u_{k1}) - (\bar{L}u_{k0}, u_{k0})] g_k^2$ is maximum to satisfy

$$\mu_q = \min I(\boldsymbol{u}) = I(\boldsymbol{u}_0) - \varepsilon^2 \sum_{k=1}^{q} w_k. \tag{9}$$

In order to select u_{k1}, we also set

$$\lambda_k = \lambda_{k0} + \varepsilon \lambda_{k1}. \tag{10}$$

Substitute (4) and (10) into (1), and equate coefficients of the same power of ε to get

$$\bar{L}u_{k0} = \lambda_{k0} u_{k0}, \quad u_{k0}|_{\partial\Omega} = 0, \tag{11}$$

$$\bar{L}u_{k1} - \lambda_{k0} u_{k1} = -\frac{p_k}{g_k} f(\rho_0) u_{k0} + \frac{p_k}{g_k} \lambda_{k1} u_{k0}, \quad u_{k1}|_{\partial\Omega} = 0. \tag{12}$$

As (11) is solvable and its solution yields the eigenfunctions ϕ_{kn} corresponding to the eigenvalues γ_{kn}, $n = 1, 2, \cdots$, and $\gamma_{km} \neq \gamma_{kn}$ if $m \neq n$, the eigenfunctions $\{\phi_{kn}\}$ form an orthonormal set so that $(\phi_{kn}, \phi_{km}) = \delta_{nm}$. To solve (12), we expand u_{k1} in terms of the orthonormal set $\{\phi_{kn}\}$:

$$u_{k1} = \sum_{m \geq 1} \alpha_{km} \phi_{km}. \tag{13}$$

Thus u_{k1} satisfies $u_{k1}|_{\partial\Omega} = 0$ because $\phi_{km}|_{\partial\Omega} = 0$ for each m. Letting $u_{k0} = \phi_{kn}$ and $\lambda_{k0} = \gamma_{kn}$, and substituting (13) into (12), by the orthonormality condition, we have

$$\alpha_{km} = \begin{cases} -\dfrac{1}{\gamma_{km} - \gamma_{kn}} \dfrac{p_k}{g_k} \displaystyle\int_\Omega f(\rho_0) \phi_{kn} \phi_{km} \mathrm{d}\Omega, & m \neq n, \\ 0, & m = n, \end{cases}$$

$$\lambda_{k1} = \int_\Omega f(\rho_0) \phi_{kn}^2 \mathrm{d}\Omega.$$

Theorem. Under the secondary approximation, the partial eigenvalue sum to problem (1) is determined by

$$\mu_q = \min I(\boldsymbol{u}) = I(\boldsymbol{u}_0) - \varepsilon^2 \sum_{k=1}^{q} [(\bar{L}u_{k0}, u_{k0}) - (\bar{L}u_{k1}, u_{k1})] g_k^2, \tag{14}$$

where $u_{k0} \in H_{0q}^1(\Omega)$, $u_{k1} \in (H_{0q}^1(\Omega))^{\perp}$, $p_k^2 + (\varepsilon g_k)^2 = 1$, $\varepsilon^3 g_k^2 < 1$, u_{k1} and g_k are determined by (8) and (13).

3 Numerical experiments

Here, we consider a system of multi-particles in the inifinitely deep potential well. Let $L = -\Delta$, $V(x) = 0$, $f(\rho) = \rho$, then problem (1) can be written as

$$\begin{cases} -\Delta u_k + \varepsilon \sum_{j=1}^{q} u_j^2 u_k = \lambda_k u_k, \quad k = 1, 2, \cdots, q, \\ u_k \mid_{\partial\Omega} = 0. \end{cases}$$

In one dimension: set $\Omega = [0,1]$, $u_{k0} = \sqrt{2}\sin k\pi x$, then

$$\bar{\mu}_q = \frac{q(q+1)(2q+1)}{6}\pi^2 + \varepsilon q\left(q + \frac{1}{2}\right) - \frac{\varepsilon^2}{8\pi^2}\sum_{k=1}^{q}\left[3\sum_{j=1, j\neq k}^{q}\frac{1}{j^2 - k^2} + 2\sum_{m=q+1}^{N}\frac{1}{m^2 - k^2}\right].$$

Table 1 shows a comparison between $\overline{\mu_q}$ and $\tilde{\mu}_q$ obtained by the ordinary method.

Table 1 Comparison between $\bar{\mu}_q$ and $\tilde{\mu}_q$

q	$\bar{\mu}_q$	$\tilde{\mu}_q$
2	54.3247790	54.3326175
5	570.3016974	570.3153740
10	3904.7707760	3904.7883036

We computed the density function $\bar{\rho}$ corresponding to $\bar{u}_k$ as shown in Figure 1.

In two dimensions: set $\Omega = [0,1] \times [0,1]$, $u_{k0} = \sin km\pi x \sin jn\pi y$, then

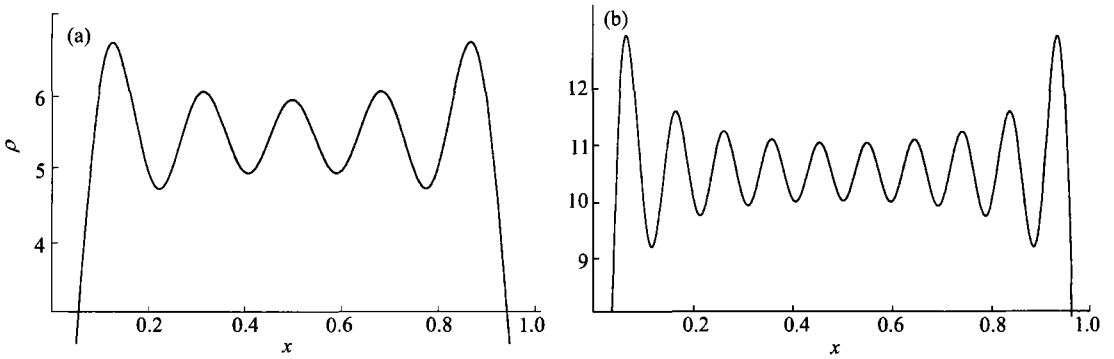

Fig. 1 Density function for $q = 5$ (a) and $q = 10$ (b).

$$\hat{\mu}_q = \frac{q(q+1)(2q+1)}{6}\pi^2(m^2+n^2) + \frac{\varepsilon q}{4}\left(q+\frac{5}{4}\right)$$

$$-\frac{\varepsilon^2}{256(m^2+n^2)\pi^2}\sum_{k=1}^{q}\left[3\sum_{j=1,\,j\neq k}^{q}\frac{1}{j^2-k^2}+2\sum_{r=q+1}^{N}\frac{1}{r^2-k^2}\right].$$

This formula can deal with the energy sum in different bands for the multi-particles on a rectangle. Fig. 2 shows the density function for single particle at ground state. Table 2 gives the values of $\hat{\mu}$ for $m, n = 1$ or 2.

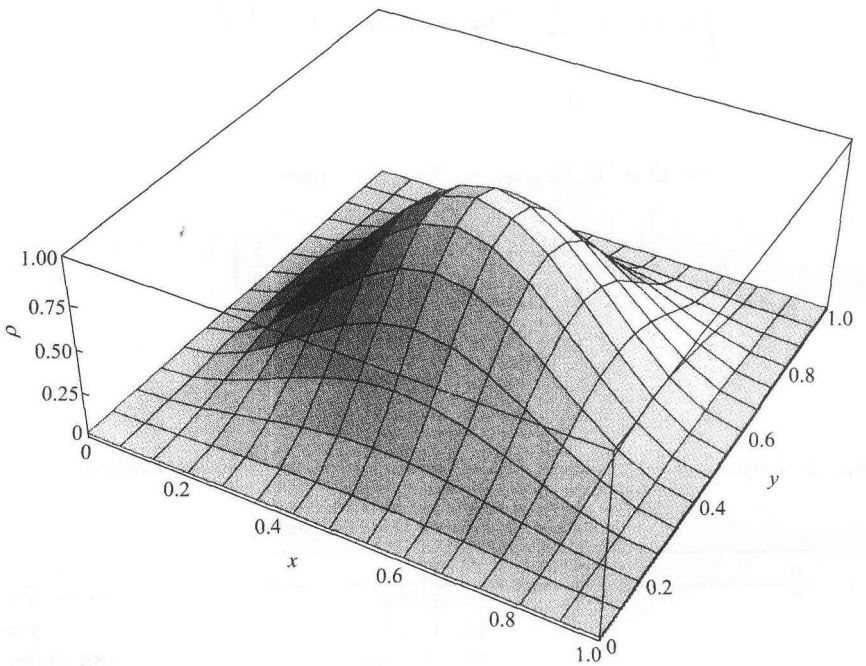

Fig. 2 Density function for single particle at ground state.

Table 2 Values of $\hat{\mu}_q$ in a rectangular domain

m, n	$q = 2$	$q = 5$	$q = 10$
$m = 1, n = 1$	100.32068	1093.46857	7627.71997
$m = 1, n = 2$	348.68565	3815.42211	26654.83327
$m = 2, n = 2$	993.45969	10887.81399	76108.45303

Acknowledgements The authors would like to thank Prof. Wang Dingsheng for his helpful discussions and valuable suggestions throughout this work.

References

1 Sun, J. C. et al. Parallel algorithm for generalized matrix eigen-problem and its application in calculation of crystal electronic structure. Chinese Science Bulletin, 1997, 42(13): 818.

2 Struwe, M. Variational Methods. New York: Springer-Verlag. 1990.

3 Jiang, M. R. et al. Minimization and error estimates for a class of the nonlinear Schrödinger eigenvalue problems. Comm. Nonli. Sci & Numer. Simul., 2000, 5(2): 80.