Indian J. pure appl. Math., 22(5): 361-368 May 1991

ON THE EXISTENCE OF AN EIGENFUNCTION OF THE HARTREE OPERATOR OF THE HELIUM ATOM BY THE FIXED POINT PRINCIPLE

RABINDRA NATH SEN

Department of Applied Mathematics, University College of Science
92, A.P.C. Road, Calcutta 700 009

AND

SHYAMAL KUMAR DUTTA

Department of Mathematics, Karimpur Pannadevi College
Nadia, West Bengal

(*Received* 19 *March* 1990; *after revision* 14 *December* 1990; *accepted* 8 *January* 1991)

In this note we apply Krasnoselskii's fixed point theorem to find the range of values of λ for which the Hartee operator for Helium atom admits of an eigen function. Earlier Reeken proved the existence of a pointwise eigen function by applying bifurcation analysis.

1. INTRODUCTION

The Hartee equations (Bazley[1]) have long been used by physicists to approximate complicated atomic and molelcular system.

They replace the linearized Schrödinger equation by a coupled system of nonlinear equations which can be solved by iterative techniques. Hartree equations form a system of non-linear differential integral equations.

In what follows we consider the simplest case of an equation namely Hartree operator for Helium under the assumption that both electrons are in identical states. Our interest is essentially mathematical. We investigate the problem of the existence of an eigenfunction.

The existence proof are roughly of the three kinds: monotonicity (i.e. positive invertibility), fixed point (i.e. iterative – compact) and variational (i.e. lower semicontinuity) (Gustafson[6]).

The existence theory for the nonlinear Hartree equation started in the dissertation of Gustafson[5]. But Zwahlen, Reeken and Bazley were the first to use functional analysis to investigate the Hartree equation. Bazley and Zwahlen[3] showed that bounded solutions bifurcate. Gustafson and Sather[7] used monotonicity property to obtain the solution for large charge. Reeken[10] proved the existence of an isolated and pointwise eigenfunction for the radial equation. Wolkowisky[12] proved the existence of a solution for excited states by using the Schauder-Tychonoff fixed point principle. Stuart[11] added his treatment with emphassis on the existence of an infinite number of excited states. Later on Bazley and Seidel[2] and Lieb and Simon[9] approached the problem variationally. One is referred to the paper by Gustafson[6] for a more detailed and systemetic exposition.

We have applied Krasnoselskii's fixed point theorem[8] to establish the existence of an eigenfunction for the Hartree operator for Helium under the assumption that both electrons are in identical states and to indicate the range of values of λ within which the corresponding eigenvalues lie. In section 2 we state the eigenvalue problem and in section 3 we present the main existence theorem based on Krasnoselskii's fixed point theorem.

2. The Eigenvalue Problem

Let us consider the real Hilbert space $H = L^2(R^3)$. In atomic units we define the Hartree operator by

$$Au = -\frac{1}{2}\nabla^2 u - \frac{2u(x)}{|x|} + u(x)\int \frac{u^2(y)\,dy}{|x-y|} \qquad \ldots(2.1)$$

where x and y denote vectors in R^3 (Bazley). Each solution to the eigenvalue problem $Au = \lambda u$ is required to satisfy the normalized condition,

$$\|u\|^2 = \int_{R^3} u^2(y)\,dy = 1 \qquad \ldots(2.2)$$

and regularity at infinity.

We also assume that $u(x)$ remains finite in the neighbourhood of the origin.

Let us assume that $u(x) = U(r)\,P_n(\theta, \phi)$ where (r, θ, ϕ) denotes the spherical polar coordinates of the point x.

We note that

$$I = \int_0^\infty \frac{u^2(y)}{|x|}\,dy$$

$$= \int_0^\infty\int_0^{2\pi}\int_0^{2\pi} \frac{U^2(r)\,r^2\,P_n^2(\theta,\phi)\sin\theta\,dr\,d\theta\,d\phi}{|r^2 + r'^2 - 2rr'\gamma|^{1/2}}$$

where, $\gamma = \mu\mu' + [(1-\mu^2)(1-\mu'^2)]^{1/2}\cos(\phi - \phi')$

$\mu = \cos\theta,\ \mu' = \cos\theta'$

Thus $$I = 4\pi\left(\frac{1}{r}\int_{r'<r} U^2(r')\,r'^2\,dr' + \int_{r'>r} U^2(r')\,r'dr'\right) f(n)$$

$$= f(n)\,q_U(r) \text{ (say)}.$$

Multiplying both sides of (2.1) by P_n (θ, ϕ) and integrating over the unit sphere we obtain

$$-\frac{1}{2r^2}\frac{d}{dr}\left(r^2\frac{dU(r)}{dr}\right) = 2\left(\lambda - \frac{2}{r} - \frac{n(n+1)}{r^2}\right)U(r) - f(n)\, q_U(r)\, U(r) \qquad \ldots(2.4)$$

where $4\pi \int_0^\infty U^2(r)\, r^2\, dr = 1$

and $U(r) \to 0$ as $r \to \infty$.

3. Existence of Eigenvalue

Let us assume that

$$BU = -\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dU}{dr}\right) + U(r) \qquad \ldots(3.1)$$

$$CU = 4\left(\frac{1}{4} + \lambda - \frac{2}{r} - \frac{2(n+1)}{r^2}\right)U(r) \qquad \ldots(3.2)$$

$$DU = -2f(n)\, \tilde{q}_U(r)\, U(r). \qquad \ldots(3.3)$$

We may note that B is a self-adjoint coercive operator[4] so that B^{-1} exists and is bounded.

However,

$$(BU, U) = 4\pi\left[-\int_0^\infty \frac{d}{dr}\left(r^2\frac{dU}{dr}\right)U(r)\, dr + \int_0^\infty r^2 U^2(r)\, dr\right]$$

$$= 4\pi\left[\int_0^\infty r^2\left(\frac{dU}{dr}\right)^2 dr + 1\right]\frac{\|U\|^2}{4\pi}.$$

Thus, $$\|BU\| \geq \left[1 + \int_0^\infty r^2\left(\frac{dU}{dr}\right)^2 dr\right]\|U\|.$$

Hence,

$$\|B^{-1}U\| \leq \|U\|. \qquad \ldots(3.4)$$

Operating on both sides of eqn. (2.5) with B^{-1} we have,

$$U(r) = \frac{4}{4\pi}\int_0^\infty \frac{e^{-\rho}}{\rho}\left[\frac{1}{4} + \lambda - \frac{2}{r'} - \frac{n(n+1)}{r'^2}\right]U(r')\, r'^2\, dr'$$

$$-\frac{2}{4\pi}\int_0^\infty \frac{e^{-\rho}}{\rho}\left[q_U(r')\, U(r')\right] r'^2\, dr' \qquad \ldots(3.5)$$

where $\rho = [r^2 + r'^2 - 2\, r\, r' \operatorname{Cos}(r, \hat{r}')]^{1/2}$

Let us denote,

$$T_1 U = 4B^{-1}\left(\frac{1}{4} + \lambda - \frac{2}{r} - \frac{n(n+1)}{r^2}\right) U(r) \qquad ...(3.6)$$

$$T_2 U = -B^{-1}(q_U(r)\, U(r)). \qquad ...(3.7)$$

Let, $U_1(r)$ and $U_2(r)$ be two functions belonging to the domain of definition of B satisfying the normalization condition and boundary condition,

Then $\| T_1 U_1(r) - T_1 U_2(r) \|$

$$= 4 \left\| B^{-1}\left(\frac{1}{4} + \lambda - \frac{2}{r} - \frac{n(n+1)}{r^2}\right)(U_1 - U_2)\right\|$$

$$\leq 4 \|B^{-1}\| \left(\left|\frac{1}{4} + \lambda\right| \|U_1 - U_2\| + 2 \left\| \frac{U_1 - U_2}{r} \right\| + n(n+1) \left\| \frac{U_1 - U_2}{r^2} \right\| \right) \qquad ...(3.8)$$

$$\leq 4 \left(\left|\frac{1}{4} + \lambda\right| \|U_1 - U_2\| + 2 \left\| \frac{U_1 - U_2}{r} \right\| + n(n+1) \left\| \frac{U_1 - U_2}{r^2} \right\| \right). \qquad ...(3.9)$$

Let us define the graph norm $\|W\|'_{\tilde{B}}$ by

$$\|W\|'_{\tilde{B}} = \alpha \left\| \frac{1}{r^2} \frac{d}{dr}\left(r^2 \frac{dW}{dr}\right) \right\| + \beta \|W\|, \ \forall\ W(r) \in D_{\tilde{B}}$$

where, $$\tilde{B} = -\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dW}{dr}\right), \ \alpha, \beta > 0.$$

It may be noted that $W(r) \in D_{\tilde{B}}$ are bounded in terms of the graph norm (Kato[13]) i.e. $\|W(r)\| \leq \gamma \|W_{\tilde{B}}\|$.

Lemma 3.1 — Let us consider a subset D_0 of the domain of B with the following properties :

For any $U_1, U_2 \in D_0$

(i) $|U_1 - U_2| \leq \beta_1 r^3$ in the neighbourhood of the origin i.e. for $r \in [0, r_0]$, r_0 small

(ii) U_1 and U_2 differ by $1/r$ in the neighbourhood of ∞ i.e. $r \in [R_0, \infty)$, R_0 large,

(iii) $\underset{0 \leq r < \infty}{\operatorname{Max}} |U(r)| \leq r_1$

Then the closure of D_0 is a closed and bounded set.
The proof is simple.

Let, $K = \{ W(r) / W(r) \in D_{\tilde{B}}, \lim_{r \to \infty} W(r) = 0$

$\| W(r) \|_{\tilde{B}} < \infty, \| W(r) \| \leq \delta, \delta < 1 \}$

so that K is a closed bounded convex set. Therefore, $K \cap [D_0]$ is closed, bounded and convex.

Thus, for $U_1, U_2 \in K \cap [D_0]$

$$\left\| \frac{U_1 - U_2}{r^2} \right\|^2 = \int_0^\infty \frac{(U_1 - U_2)}{r^2} dr \leq \| U_1 - U_2 \|^2 \left\| \frac{U_1 - U_2}{r^4} \right\|^2 \qquad \ldots(3.10)$$

Also,

$$\left\| \frac{U_1 - U_2}{r} \right\| \leq \| U_1 - U_2 \| \left\| \frac{U_1 - U_2}{r^2} \right\| \qquad \ldots(3.11)$$

Using (3.10) and (3.11), (3.9) further reduces to

$$\| T_1 U_1 - T_1 U_2 \| \leq 4 \left(\left| \frac{1}{4} + \lambda \right| + 2 \left\| \frac{U_1 - U_2}{r^2} \right\| + n(n+1) \left\| \frac{U_1 - U_2}{r^4} \right\| \right) \| U_1 - U_2 \|$$

Lemma 3.2 – T_1 is contractive in $L_2 (0, \infty)$ norm in $K \cap [D_0]$ if,

$$4 \left[\left| \lambda + \frac{1}{4} \right| + 2 \left(\frac{\beta^2 r_0^5}{5} + \frac{4\gamma^2}{R_0} \right)^{1/2} + n(n+1) \left(\beta^2 r_0 + \frac{4\gamma^2}{5R_0^2} \right)^{1/2} \right] < 1. \qquad \ldots(3.12)$$

Proof : For $U_1, U_2 \in \tilde{K}$ ($= K \cap [D_0]$)

$$\left\| \frac{U_1 - U_2}{r^2} \right\|^2 = \int_0^\infty \frac{U_1 - U_2}{r^2} dr \leq \frac{\beta^2 r^5}{5} + \frac{4\gamma^2}{R_0}$$

Similarly, $$\left\| \frac{U_1 - U_2}{r^4} \right\|^2 \leq \beta^2 r_0 + \frac{4\gamma^2}{5R_0^5}$$

Thus, T_1 is contractive if

$$4 \left[\left| \lambda + \frac{1}{4} \right| + 2 \left(\frac{\beta^2 r_0^5}{5} + \frac{4\gamma^2}{R_0} \right)^{1/2} + n(n+1) \left(\beta^2 r_0 + \frac{4\gamma^2}{5R_0^5} \right)^{1/2} \right] < 1. \qquad \ldots(3.13)$$

Now, $q_U(r)$ is relatively compact with respct to $\tilde{B}$ (Reeken[10]). Therefore, on $\tilde{K}$, DU is completely continuous. B^{-1} being a bounded linear operator, T_2 is a compact operator on $\tilde{K}$ and is continuous too.

Lemma 3.3 – Let the following conditions be fulfilled :

(i) $\forall U(r) \in \tilde{K}$, α is sufficiently small

(ii) $$\int_1^\infty U^2(r)\, r^2\, dr \geq \int_1^\infty U^2(r)\, dr + \int_0^1 U^2(r)\, dr - \int_0^1 U^2(r)\, r^2\, dr$$

(iii) $$\int_1^\infty U^2(r)\, dr \geq \int_1^\infty \frac{U^2(r)}{r^2}\, dr + \int_0^1 \frac{U^2(r)}{r^2}\, dr - \int_0^1 U^2(r)\, dr$$

(iv) $$\int_1^\infty \frac{U^2(r)}{r^2}\, dr \geq \int_1^\infty \frac{U^2(r)}{r^6}\, dr + \int_0^1 \frac{U^2(r)}{r^6}\, dr - \int_0^1 \frac{U^2(r)}{r^2}\, dr$$

(v) $$4\left\{\left|\frac{1}{4} + \lambda\right| + 2\delta + n(n+1)\delta + \pi C_2' \delta\right\} \leq 1.$$

The. ˆ $U(r), V(r) \in \tilde{K}$, $T_1 U(r) + T_2 V(r) \in \tilde{K}$.

Proof : For all $U(r) \in \tilde{K}$.

$$\|T_1 U(r)\| \leq 4\left[\left|\frac{1}{4} + \lambda\right| + 2\left\|\frac{U(r)}{r^2}\right\| + n(n+1)\left\|\frac{U(r)}{r^4}\right\|\right]\|U(r)\|. \qquad ...(3.14)$$

By virtue of conditions (ii) and (iii)

$$\left\|\frac{U(r)}{r^2}\right\|^2 = \int_0^\infty \frac{U^2(r)}{r^2}\, dr \leq \int_0^\infty U^2(r)\, dr \leq \int_0^\infty U^2(r)\, r^2\, dr.$$

Similarly by (iv)

$$\left\|\frac{U(r)}{r^4}\right\|^2 \leq \int_0^\infty U^2(r)\, r^2 = \|U(r)\|^2.$$

Thus, $$\|T_1 U(r)\| \leq 4\left[\left|\frac{1}{4} + \lambda\right| + 2\delta + n(n+1)\delta\right]\|U(r)\|. \qquad ...(3.15)$$

Now, for $V(r) \in \tilde{K}$

$$0 \leq q_V(r) \leq 4\pi C_2' \|V(r)\| \|V(r)\|_{\tilde{B}} \text{ (Reeken[10])}.$$

Therefore for $V(r) \in \tilde{K}$,

$$\|q_V(r)\ V(r)\| \leq 4\pi\ C_2'\ \delta\ \|V(r)\|_{\tilde{B}}. \qquad \ldots(3.16)$$

From (3.15) and (3.16) we conclude for $U(r),\ V(r) \in K$,

$$\|T_1\ U(r) + T_2\ V(r)\| \leq \left[4\left\{\left|\frac{1}{4} + \lambda\right| + 2\delta + n\ (n+1)\ \delta\right\} + 4\pi\ C_2'\ \delta\ \|V(r)\|_{\tilde{B}}\right]\delta. \qquad \ldots(3.17)$$

Keeping in mind that α is sufficiently small and using condition (V) we infer that

$$T_1\ U + T_2\ V \in \tilde{K}\ \forall\ U(r),\ V(r) \in \tilde{K}.$$

We now state below Kransnoselskii's fixed point theorem (Rall[14]).

Theorem 3.1 – (Krasnoselskii[8]) – Let T_1 and T_2 be operators which are defined in a bounded, closed couvex set C of a Banach R and suppose

(i) $T_1\ U + T_2\ V \in C$ for every pair $U,\ V \in C$,

(ii) T_1 is contractive i.e. there exists a constant $\mu < 1$ with

$$\|T_1 U - T_1 V\| \leq \mu\ \|U - V\|$$

for all $U,\ V \in C$,

(iii) T_2 is completely continuous.

Then there exists atleast one fixed point

$U^* \in \tilde{K}$ which satisfies

$U^* = T_1\ U^* + T_2\ U^*.$

Taking scalar product of both sides of eqn. (2.1) with $u(x)$ we may note that

$$-\frac{1}{2}\ (u,\ \nabla^2 u) - 2\left(\frac{u}{|x|},\ u\right) + \left(u(x)\int \frac{u^2\ (y)}{|x-y|}\,dy,\ u(x)\right) = \lambda\ (u(x),\ u(x))$$

showing that λ is real.

Theorem 3.2 — Equation (2.1) will have an eigenvalue λ and hence will admit of an eigenfunction (spherically symmetric) if

λ satisfies (3.13), condition and (iv) of Lemma 3.3 and

$$\left|\lambda + \frac{1}{4}\right| < \text{Min}\left[\frac{1}{4} - 2\left(\frac{\beta^2 r_0^5}{5} + \frac{4\gamma^2}{R_0}\right)^{1/2} - n\ (n+1)\left(\beta^2 r_0 + \frac{4\gamma^2}{5R_0^5}\right)^{1/2} \right.$$

$$\left. \frac{1}{4} - (2 + n\ (n+1) + \pi\ C_2')\ \delta\right]. \qquad \ldots(3.18)$$

The theorem is proved by making an appeal to Lemmas 3.1 to 3.3 and Krasnoselskii's fixed point theorem.

It may be noted that (3.18) gives a quantitative estimate of the range of values of λ for which equation (2.1) will admit of an eigenfunction.

ACKNOWLEDGEMENT

The authors are grateful to the referee for his valued suggestions.

REFERENCES

1. N. W. Bazley, Existence and Bounds For the Lowest Critical Energy of the Hartree Operator, *Lecture Notes in Mathematics* (ed. : B. D. Sleeman and I. M. Michael), Springer Verlag, 1974.
2. N. Bazley and R. Seidel, *Chem. Phys. Lett.* **24** (1974), 128-32.
3. N. Bazley and B. Zwahlen, *Manuscripta Math.* **2** (1970), 365-74.
4. J. Cea, *Lecture Notes on Optimization, Theory and Algorithm*, TIFR, Narosa, 1978.
5. K. Gustafson, DISSERTATION, IFDAM Technical Note BN-389, 1965.
6. K. Gustafson, *Recent Progress on the Nonlinear Hartree-Fock, Concentration-Diffusion and Navier-Stokes Equations, Conference Proceedings*. (ed: Amann, Kirchgassner and Bazley), 1979.
7. K. Gustafson and D. Sather, *Rendiconti di Math.* **4** (1971), 723-34.
8. M. A. Krasnoselskii, *U.M.N.* **10** (1955), 123-27.
9. E. Lieb and B. Simon, *Commun. Math. Phys.* **53** (1977), 185-94.
10. M. Reeken, *J. Math. Phys.* **2** (1970), 205-12.
11. C. Sturt, *Archiv Ration Mech. Anal.* **51** (1973) 60-69.
12. J. Wolkowisky, *Indiana Univ. Math.* **22** (1922) 551-558.
13. T. Kato, *Perturbation Theory for Linear Operators* Springer-Verlag, 1966.
14. L. B. Rall (ed.), *Some Application of Functional Analysis to Analysis, Particularly to Non-Linear Integral Equations*, 1971.