Stobility of Motter p. 16

24 Jour whise in TF theory

25 Howman - Foch the ory

24. Ionization in TF theory

What we sis not prove exactly but what is true about the Thomas-Ferri functional is the foll - wing :

The (Existence of TF minimis) Lot $D_{N} = 3geL' n L^{r_{3}} | g \ge 0$, $Sg \le N S$

There exists Sr EDN such that

 $inf \in \mathcal{E}^{TF}(g) = \mathcal{E}^{TF}(g*)$

The proof is a problem in collectus of veriations so we omit the proof.

Z

It times out the minimizer is olso canique

which fillows from converity:

 $\mathcal{E}^{TF}(\lambda_{r}+(\Lambda-\lambda_{s}) \leq \lambda \mathcal{E}^{TF}(q) + (\Lambda-\lambda) \mathcal{E}^{TF}(q)$

for Sirgi E DN and ZE C>11.

Another consequence of converts is that for Si - minimum N PN, and Si - minimum in PN, we have

 $E_{\lambda N_{1}+(A-\lambda | N_{1})} \leq E^{TF}(\lambda_{g, +(A, \lambda)} P_{1}) \leq \lambda \in T^{F}(g,) + (A \cdot A) \in T^{F}(g_{1})$

 $= \lambda E_{N_{1}}^{TF} + (\Lambda \cdot \lambda) E_{N_{1}}^{TF}$

which Shows

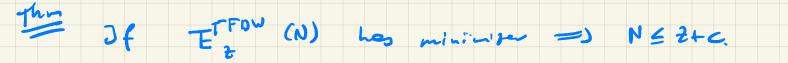
Lemme The ground shoke every of EN is convex, nonincreasing and banded from bolow (as a fit of N) Thus the kinit $\lim_{N \to \infty} E_N^{TE} = E_\infty$ exists. Ve Befine $N_e := i - f + N + E_N^{TF} = E_A$. We do not know yet whether Ne 200. Let Ju = 1 geon : Sp=NS. The next theorem characterises the shape of EN. Theorem For NENC, there exists a unique minimiter of ETF in Jr. The function ENF is strictly convex and decreasing in [O, N.J. If NCCO and NSNe, then there is no minimited on Fr. The function greats the unique minimizer in Op. Korean, Er is constant in [Ne, ...)-Thus, Ne is the largest number of dectrons san

that there is a minimiter - ionitation conjective?

It turns art that in Thomas - Fermi thoong we hove Theorem $N_c = Z$ 24.1 Thomas - Farmi - von Weitsäcken (TFN) then In principle: TF purchy classical and good to describe bulk of electrons of dirtome O(2") for the nucleus. For physical and aread epplications it is impohent to capture contributions from concrust and outermost dechons of Hirtonecs O(t-1) and O(1). ~ refinements $\mathcal{E}^{TFW}(u) = \int \left(C^{TF} |u|^{10/3} + C^{W} |\nabla u|^{2} - \frac{2|u|^{2}}{|u|} + \frac{1}{2} |u|^{2} \left(|u|^{2} \frac{1}{|u|} \right) \right)$ $\frac{|u|^{2}}{|u|^{2}}$ $E^{TFW}(N) = \inf_{\|Lu\|_{2}^{2}=N} E^{TFW}(w)$ 1412 - vole of electron density and the ron Weizsächen correction for a contract with corresponds to the contradiction of the innernost dectrons.

In the context of the isnisotion conjecture The vertetional problem $E^{TPW}(N)$ has a minimizer $Off \quad N \leq N_c C_c^2$ with $Z \leq N_c C_c^2 \leq Z + C.$

Other extensions TFDW theory (D for Divac) - co S S (4) "3 additional tem 103



25. Howtwee- Foch thoong

E^{HF} := inf < p, HN ~p> ~p- Slater determinents

dived term As dready served last time:

Ju fout:

Exercise : Show that

S(x) S(y) - 18(x,y) 12 30 4x, yrin"

recall, By Condy - Schwern $|\{\zeta(u_i)\}| \leq \sum_{i=1}^{N} |u_i(u_i)| |u_i(v_i)| \leq \left(\sum_{i=1}^{N} |u_i(u_i)|^2\right) \left(\sum_{i>1}^{N} |u_i(v_i)|^2\right)$

=) 18(x,2)12 = So(~) Sr(2) J.

Thus the Hortnee-Fach energy can be newvilter as

$$E^{\mu F} = i \cdot F \quad \Xi^{\mu F} (y)$$

$$O(y) = y' < 1$$

$$T_{y} = N$$

Here the condition j=y2 is to ensure that y is a projection. For some computations it is more convenient to ignore this condition. Since the set 20 ≤ y ≤ 1, T-y=N y is convex.

Actually it is possible to do that without losing anything, privided that the intervalion potenshial is non-negotive.

The (Lich's veristional principle) If w30, then EHF = inf EHF(y). OEYEL Try=N (Henre V is supposed to be megalor eneo-yh) B Ju some situations : reduced Kortnee - Foch: $E^{nHF} = i_{n}f \cdot E^{nHF}$ $O \leq g \leq 1$ $T_{n}g = N$ ENHF(y) = Tro ((-h'o +V)y) + A SS (n)g(y) w(v-y)dagy Thus, keep Birect town, igne the codage ten. Mothematically coster to endyte since of 320 then you Envery is cause. Also if w20 $E_N \leq E^{M^2} \leq E^{-M^2}$ Atomic case: (HN- semi-classice mean-field) $E_{N} = -c_{1}N + c_{2}N'' - c_{2}N'' + o(N'')_{N''}$ TF theory ISZO'S) Siedentrop-(Live - Simon 1820'S) - Weilcond 1820

- Veilcond (S?)