Hugenholtz-Van Hove Theorem for Multi-Component Fermi Systems with Multi-body Forces

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Introduction

The Hugenholtz-Van Hove(HVH) theorem [1] deals with the single-particle properties of an interacting infinite Fermi system at absolute zero of temperature relating three fundamental physical quantities namely, the average energy per fermion E/A, the pressure of the system and the Fermi energy ϵ_f as

$$\frac{E}{A} + \rho \frac{\partial(E/A)}{\partial \rho} \mid_\Omega = \left(\frac{\partial E}{\partial A}\right)_\Omega, \qquad (1)$$

where ρ and Ω are respectively the number density and volume of the system. Hugenholtz and Van Hove also showed $\left(\frac{\partial E}{\partial A}\right)_\Omega = \epsilon_f$. leading to the theorem

$$\frac{E}{A} + \rho \frac{\partial(E/A)}{\partial \rho} \mid_\Omega = \epsilon_f. \qquad (2)$$

The second term being the pressure of the system would vanish for a saturating system at ground state *i.e.* at equilibrium resulting in the Eq. $E/A = \epsilon_f$. This is a rare theorem in many-body Physics, which has been rigorously shown[1] to be true by its original authors Hugenholtz and Van Hove by taking all orders of perturbation in the frame-work of time-independent perturbation theory[1–5]. However it should be mentioned here that prior to this rigorous proof Bethe[6] had also visualized the theorem under HF approximation. It is valid for any interacting infinite Fermi system and thereby applicable to liquid ^3He and in particular to nuclear matter. With its help Hugenholtz and Van Hove could find[1] internal inconsistencies in the early nuclear matter calculations of Brueckner [7]. Apart from its utility otherwise, Hugenholtz and Van Hove while proving the theorem have clearly brought out the physical meaning associated with the single particle states of an interacting many-fermion system.

The theorem has been recently extended [8] to asymmetric nuclear matter, which was then used for constructing a successful mass model well-known in the literature as the infinite nuclear matter (INM) model of atomic nuclei[9–12]. However the question of its validity in the presence of multi-body interaction terms remains unanswered. Similarly its extension to multi-component Fermi systems would be extremely useful.

HVH Theorem with Multi-body Forces

For this we follow Bethe[6] in adopting HF approximation. Taking the effective interaction for a many-body system to include all possible multi-body interaction terms $G_2, G_3, G_4, ..., G_n$ etc., the single-particle energy ϵ_i and the total energy E of the system under HF approximations are

$$\begin{aligned}\epsilon_i &= < i \mid -\frac{\hbar^2}{2m}\nabla^2 \mid i > + \sum_j < ij \mid G_2 \mid ij > \\ &+ .. + \frac{1}{(n-1)!}\sum_{j..n} < ij..n \mid G_n \mid ij..n > \qquad (3)\end{aligned}$$

and

$$\begin{aligned}E &= \sum_i < i \mid -\frac{\hbar^2}{2m}\nabla^2 \mid i > + \frac{1}{2}\sum_{ij} < ij \mid G_2 \\ &\mid ij > + .. + \frac{1}{n!}\sum_{i..n} < i..n \mid G_n \mid i..n > \qquad (4)\end{aligned}$$

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where $\mid i>, \mid j>$ etc. represent the occupied single particle states and $< i..n \mid G_n \mid i..n >$ denote the antisymmetric many-body matrix elements with the multi-body interaction G_n. For an infinite Fermi system, the above Eqs. can be further simplified as

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m} + \frac{\Omega}{(2\pi)^3} \int_0^{k_f} < kk' \mid G_2 \mid kk' > d^3k' + ... + \frac{1}{(n-1)!} \Big[\frac{\Omega}{(2\pi)^3}\Big]^{n-1} \int_0^{k_f} ... \int_0^{k_f} < kk_2..k_n \mid G_n \mid kk_2..k_n > d^3k_2..d^3k_n \quad (5)$$

and

$$E = \frac{\Omega}{(2\pi)^3} \int_0^{k_f} \frac{\hbar^2 k^2}{2m} d^3k + \frac{1}{2}\Big[\frac{\Omega}{(2\pi)^3}\Big]^2 \int_0^{k_f} \int_0^{k_f} d^3k d^3k' < kk' \mid G_2 \mid kk' > +.. + \frac{1}{n!}\Big[\frac{\Omega}{(2\pi)^3}\Big]^n \int_0^{k_f} \int_0^{k_f} .. \int_0^{k_f} d^3k_1..d^3k_n < k_1..k_n \mid G_n \mid k_1..k_n > . \quad (6)$$

The total energy E/A being a function of k_f, its derivative with respect to k_f at constant Ω can be easily obtained for all the multi-body interaction terms thereby leading to the HVH theorem (Eq. 2).

Extension to Multi-Component Fermi Systems

Consider the system to consist of n types of fermions, the number of each type being $N_i, i = 1, 2, ..n$, such that the total number N is equal to $N_1 + N_2 + ... + N_n$. Defining the fractional composition f_i of a given type of fermions i by $f_i = N_i/N, i = 1, 2..n$. Then the system will have n Fermi energies given by

$$\epsilon_i^f = \left(\frac{\partial E}{\partial N_i}\right)_{\Omega, N_1, ..N_{i-1}, N_{i+1}, ..N_n}, i = 1, ..n. \quad (7)$$

As the total energy E being a function of $N_1, N_2, .., N_n$ or alternatively $N, f_1, f_2, ..f_n$, it follows that

$$\left(\frac{\partial E}{\partial N}\right)_{\Omega} = \left(\frac{\partial E}{\partial N_1}\right)_{\Omega, N_2, N_3..} \left(\frac{\partial N_1}{\partial N}\right)_{f_1} + \left(\frac{\partial E}{\partial N_2}\right)_{\Omega, N_1, N_3..} \left(\frac{\partial N_2}{\partial N}\right)_{f_2} + .. = \sum_{i=1}^{n} \epsilon_i^f f_i. \quad (8)$$

Using Eq. (1), we arrive at the most generalized form of HVH theorem as

$$\frac{E}{A} + \rho \frac{\partial(E/A)}{\partial \rho} = \sum_{i=1}^{n} \epsilon_i^f f_i, \quad (9)$$

which for ground state reduces to

$$\frac{E}{A} = \sum_{i=1}^{n} \epsilon_i^f f_i. \quad (10)$$

It is needless to mention the utility of such a generalized HVH theorem that can be applied to any multi-component Fermi system.

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