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Possibility of Abnormal Fermion Occupation in Nuclear Matter with Non-Local, Separable Interactions

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Using the $^3S_1$ part of several non-local, separable nucleon-nucleon interactions, we investigate the conditions under which abnormally-occupied plane-wave Slater determinants can have lower Hartree-Fock energy than the standard, normally-occupied one.

Usando a parte $^3S_1$ de várias interações núcleon-núcleon, não locais e separáveis, estudamos as condições sob as quais determinantes de Slater de ondas planas com ocupações anormais possam dar uma energia de Hartree-Fock menor do que a dada pela ocupação normal.

1. INTRODUCTION

The normal fermi sea unperturbed vacuum state consisting of a plane-waves determinant with all wave-number vectors occupying the fermi sphere has been the standard "starting point" about which to carry out either perturbative[1] or variational[2] correlation energy studies in the many-fermion problem. This choice is clearly the optimum one for a non-interacting fermi gas, and the possibility of other (abnormal) ways

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of occupying the zero-order state immediately suggests itself as soon as interactions are taken into account. For both N-fermion[3] and N-boson[4] matter the question has been investigated for local two-particle interactions where a possible abnormal occupation derives entirely from the exchange interaction energy. Non-local, separable potentials[5] contribute entirely through the direct interaction energy (thus providing a completely different mechanism for possible abnormal occupation) and is studied in this paper.

2. ABNORMAL OCCUPATION AND KINETIC ENERGY

If we occupy in each space - spin - isospin state $\vec{k}\sigma\tau$ of the zero-order Slater determinant of plane waves $n_{\vec{k}} = n_k$ fermions (= 0 or 1) the total number of particles N, in a box of volume V where periodic - boundary conditions are applied, is given by

$$N = \sum_{\vec{k}\sigma\tau} n_{\vec{k}} \xrightarrow[\text{large } V]{} \frac{\nu V}{(2\pi)^3} \int d\vec{k}\, n_k = \frac{\nu V}{2\pi^2} \int dk\, k^2\, n_k \tag{1}$$

$\nu \equiv \sum_{\sigma\tau} 1$ (=2, neutron matter; = 4 nuclear matter; etc). Normal occupation is defined by

$$n_k = \theta(k_F - k) \;, \tag{2}$$

where $\theta(x) \equiv \frac{1}{2}[1 + \text{sgn}(x)]$, and implies from (1) that the particle density

$$\rho \equiv \frac{N}{V} = \frac{\nu k_F^3}{6\pi^2} \;. \tag{3}$$

Abnormal occupation will be defined as

$$n_k = \theta(\alpha k_F - k) + \theta(\beta k_F - k)\,\theta(k - \gamma k_F) \quad ; \quad \alpha \geqslant 0 \quad , \; \beta \geqslant 1 \;. \tag{4}$$

There being say N_1 particles in the sphere of radius αk_F, in k-space, and N_2 in the shell of inner radius γk_F and outer βk_F, one has from (1),

$$N_1 = \nu V \alpha^3 k_F^3/(6\pi^2) = N\alpha^3 \;,$$

$$N_2 = \nu V(\beta^3-\gamma^3)k_F^3/(6\pi^2) = N(\beta^3-\gamma^3) \; ,$$

thus

$$N_1 + N_2 = N \rightarrow \alpha^3 + \beta^3 - \gamma^3 = 1 \; , \qquad (5)$$

so that only <u>two</u> (variational) parameters, say a and β, remain.

The kinetic energy expectation value in an abnormally occupied Slater determinantal state is then, using (3),

$$\langle -(\hbar^2/2m) \sum_{i=1} \nabla_i^2 \rangle = \nu \sum_{\vec{k}} (\hbar^2 k^2/2m)\, n_k = \frac{\hbar^2}{2m} \frac{\nu V}{(2\pi)^3} \left[\int_0^{\alpha k_F} dk\, k^4 + \int_{\gamma k_F}^{\beta k_F} dk\, k^4 \right]$$

$$= \frac{3}{5} N \frac{\hbar^2 k_F^2}{2m} (\alpha^5 + \beta^5 - \gamma^5) \geq \frac{3}{5} N \frac{\hbar^2 k_F^2}{2m} \; , \qquad (6)$$

where the last quantity is of course the normally - occupied determinant expectation value (ideal fermi-gas kinetic energy).

3. ABNQRMAL OCCUPATION AND POTENTIAL ENERGY

a) Direct and Exchange Potential Energias

For a potential energy $v \equiv \sum_{i<j}^{N} v_{ij}$, the expectation value is $(K_i \equiv \vec{k}_i \sigma_i \tau_i)$

$$\langle v \rangle = \frac{1}{2} \sum_{K_1 K_2} | \langle K_1 K_2 | v_{12} | K_1 K_2 \rangle - \langle K_1 K_2 | v_{12} | K_2 K_1 \rangle |\, n_{\vec{k}_1} n_{\vec{k}_2}$$

$$\equiv \langle v \rangle_{dir} - \langle v \rangle_{exch} \; . \qquad (7)$$

If the two-body potential v_{12} is of the non-local, separable type[5] then, $\vec{k}$ r $\frac{1}{2}(\vec{k}_1-\vec{k}_2)$, the direct contribution

$$\sum_{\sigma_1\tau_1\sigma_2\tau_2} \langle K_1K_2|v_{12}|K_1K_2\rangle \equiv \frac{(2\pi)^3}{V} \; v(\vec{k}|\vec{k})$$

$$\equiv \frac{(2\pi)^3}{V} \; \frac{2\hbar^2}{\pi m} \sum_{\substack{JTS \\ L'L}} v_{JTSL'L}(\vec{k}|\vec{k}) \tag{8}$$

where $JTST$ refer to two-body total, orbital and spin angular momentum, and isospin, respectively, and

$$v_{JTSL'L}(\vec{k}|\vec{k}) = f^{JTS}_{L'L}(k|k) \; \tilde{y}^{JTS}_{L'M}(\hat{k}) \; \tilde{y}^{*JTS}_{LM}(\hat{k}) \tag{9}$$

where the notation of ref.5 is being employed for the radial $f(k\;k)$ and spin-angular $y(k)$ functions. Similarly, the exchange contribution

$$\sum_{\sigma_1\tau_1\sigma_2\tau_2} \langle K_1K_2|v_{12}|K_2K_1\rangle \equiv \frac{(2\pi)^3}{V} \; v(\vec{k}|-\vec{k})$$

$$\equiv \frac{(2\pi)^3}{V} \; \frac{2\hbar^2}{\pi m} \sum_{\substack{JTS \\ L'L}} v_{JTSL'L}(\vec{k}|-\vec{k})$$

$$= \frac{(2\pi)^3}{V} \; \frac{2\hbar^2}{m} \sum_{\substack{JTS \\ L'L}} (-)^{L+S+T} \; v_{JTSL'L}(\vec{k}|\vec{k}) \tag{10}$$

where in the last step one used the identity

$$\tilde{y}^{JTS}_{LM}(-\hat{k}) = (-)^{L+S+T} \; \tilde{y}^{JTS}_{LM}(\hat{k}) \;. \tag{11}$$

Since the exclusion principle requires that $(-)^{L+S+T} = -1$, eq. (7) finally reduces to

$$\langle v\rangle = \sum_{K_1K_2} \langle K_1K_2|v_{12}|K_1K_2\rangle n_{\vec{k}_1} n_{\vec{k}_2} = 2\;\langle v\rangle_{\rm dir} \;. \tag{12}$$

Alternatively, defining $\vec{K} = \vec{k}_1 + \vec{k}_2$, one has for nuclear matter

$$\langle v\rangle/N = \frac{3\hbar^2}{8m\pi^2 k_F^3} \sum_{\substack{JTS \\ L'L}} (2J+1)(2T+1) \int dk \; k^2 \; f^{JTS}_{L'L}(k|k)$$

$$\times \int d\vec{K} \; n_{\left|\frac{1}{2}\vec{K}+\vec{k}\right|} \; n_{\left|\frac{1}{2}\vec{K}-\vec{k}\right|} \tag{13}$$

b) Overlap of Fermi Spheres and Shells

For normal occupation the last integral in (13) is the well-known[6] overlap volume in k-space of two fermi spheres, each of radius k_F and whose centers are separated by a distance $2k$ (as this is the volume that the two vectors $(\vec{K}+\vec{k})/2$ and $(\vec{K}-\vec{k})/2$ are allowed to sweep out). The standard result for $n_k = \theta(k_F-k)$ is just

$$\int d\vec{K}\, n_{|\frac{1}{2}\vec{K}+\vec{k}|}\, n_{|\frac{1}{2}\vec{K}-\vec{k}|} = \frac{32\pi}{3} k_F^3\, g(k/k_F)\,\theta(k_F-k) \quad , \tag{14}$$

$$g(x) \equiv 1 - \frac{3}{2}x + \frac{1}{2}x^3 \; . \tag{15}$$

The abnormal case (4) analogously reduces the last integral in (13) to a k-space volume overlap problem of considerable complexity. However, for $\alpha=0$ one has a single shell[3] and the overlap problem is more tractable. The overlap topologies are <u>distinct</u> depending on whether the "shell" width $\beta-\gamma$ is greater or less than the "hole" diameter 2γ (in units of k_F), giving rise to <u>two cases</u>:

$$\begin{aligned} &\text{Case I} \;:\; \beta-\gamma < 2\gamma \text{ or } \beta > (27/26)^{1/3} \sim 1.01266 \\ &\text{Case II} \;:\; \beta-\gamma > 2\gamma \text{ or } 1 \leq \beta < (27/26)^{1/3} \; . \end{aligned} \tag{16}$$

A somewhat tedious but straightforward calculations finally leads to

$$(3/32\pi k_F^3) \int d\vec{K}\, n_{|\frac{1}{2}\vec{K}\,\vec{k}|}\, n_{|\frac{1}{2}\vec{K}\,\vec{k}|} = \begin{cases} v_I(x) & \text{(case I)} \\ v_{II}(x) & \text{(case II)} \end{cases} \tag{17}$$

where $x = k/k_F$ and

$$\begin{aligned} v_I(x) \equiv\; & V_1(x)\theta(\beta-x)\theta(x-[\beta+\gamma]/2) + V_2(x)\theta(x-\gamma)\theta([\beta+\gamma]/2-x) \\ & + V_3(x)\theta(\gamma-x)\theta(x-[\beta-\gamma]/2) + V_4(x)\theta([\beta-\gamma]/2-x) \quad , \end{aligned} \tag{18}$$

$$v_{II}(x) \equiv V_1(x)\theta(\beta-x)\theta(x-[\beta+\gamma]/2) + V_2(x)\theta([\beta+\gamma]/2-x)\theta(x-[\beta-\gamma]/2)$$

$$+ \tilde{V}_2(x)\theta([\beta-\gamma]/2-x)\theta(x-\gamma) + V_4(x)\theta(y-r) \quad ; \tag{19}$$

$$V_1(x) \equiv \beta^3 g(x/\beta) \quad , \tag{20}$$

$$V_2(x) \equiv V_1(x) - [\gamma^3 g(x_A/\gamma) + \beta^3 g(x_B/\beta)] \quad , \tag{21}$$

$$V_3(x) \equiv V_1(x) - [\gamma^3 g(x_A/\gamma) + \beta^3 g(x_B/\beta) - \gamma^3 g(x/\gamma)] \quad , \tag{22}$$

$$V_4(x) \equiv V_1(x) - 2\gamma^3 + \gamma^3 g(x/\gamma) \quad , \tag{23}$$

$$\tilde{V}_2(x) \equiv V_1(x) - 2\gamma^3 \quad ; \tag{24}$$

$$x_A \equiv (\gamma^2-\beta^2+4x^2)/4x \quad , \quad x_B \equiv (\beta^2-\gamma^2+4x^2)/4x \quad , \tag{25}$$

and $g(x)$ is defined as in (15).

The potential energy difference is then

$$\Delta\langle v\rangle/N \equiv \left[\langle v\rangle_{\text{abnormal}} - \langle v\rangle_{\text{normal}}\right]\Big/N$$

$$= \frac{4\hbar^2}{\pi m} \sum_{\substack{JTS \\ L'L}} (2J+1)(2T+1) \int_0^{\beta k_F} dk\, k^2\, f^{JTS}_{L'L}(k|k)\Delta(\beta;k/k_F) \quad ,$$

$$\Delta(\beta;k/k_F) \equiv v_{I \text{ or } II}(k/k_F) - g(k/k_F)\theta(k_F-k) \quad . \tag{26}$$

The last function is plotted in Fig.1 for several values of $\beta>1$; note that it vanishes for $\beta=1$, as it should.

In the following, we study the N-fermion system with several non-local, separable two-particle interactions, but we shall limit ourselves to the $^3S_1$ state.

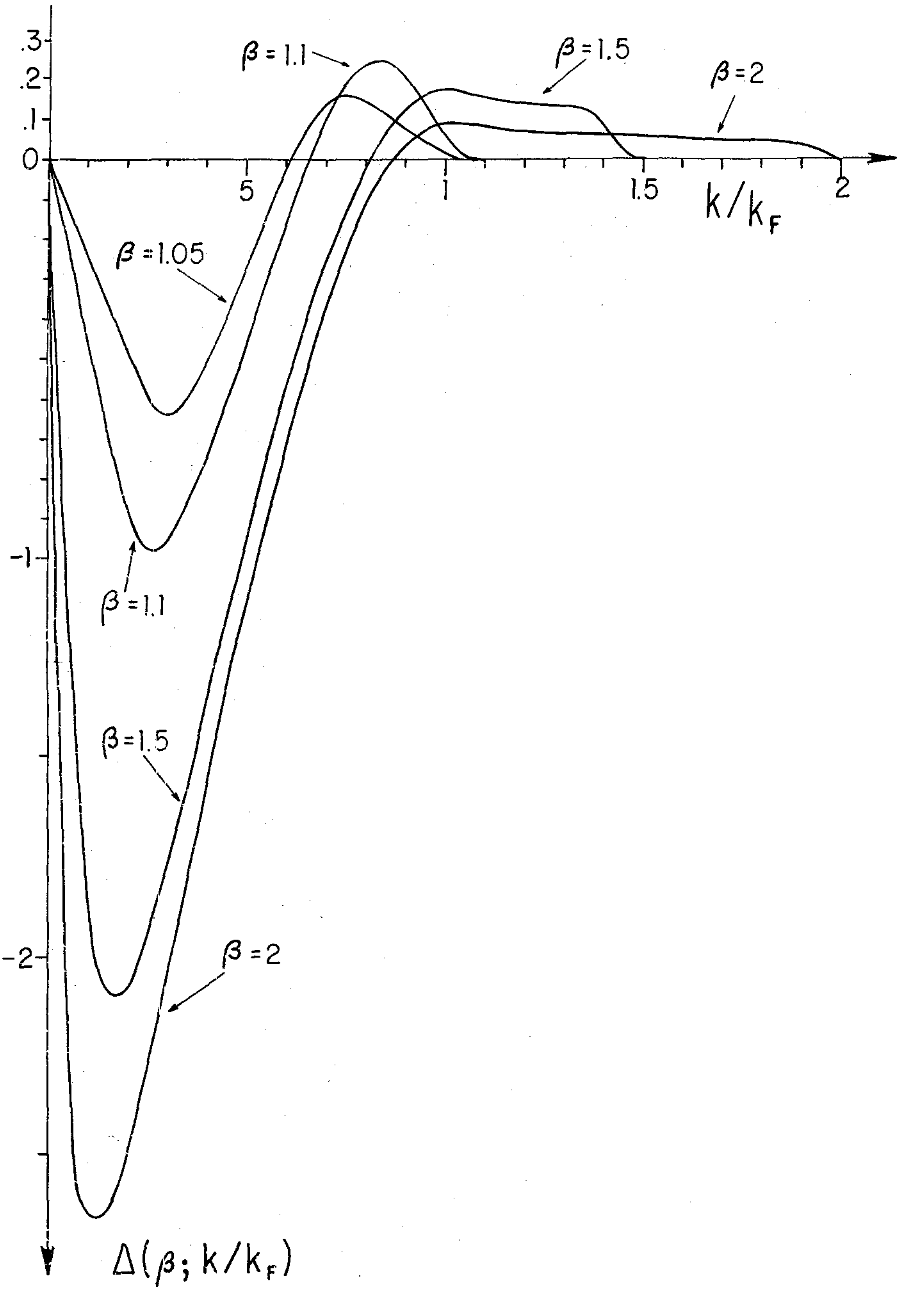

Fig.1 - The function $\Delta(\beta;k/k_F)$ defined in Eq. (26) for different values of $\beta>1$. It represents the abnormally-occupied k-space volume overlap, Eqs. (18) and (19), minus the normally occupied one, Eq. (15). Note that this difference vanishes for $\beta=1$ (normal occupation).

c) Dynamics

We have considered: i) the purely attractive portion of the Tabakin[7] interaction for which $f^{JTS}_{L'L}(k|k)$ is

$$f^{101}_{00}(k|k) = -\tilde{\gamma}^2/(k^2+a^2)^2 \quad , \tag{27}$$

$$\hbar^2\tilde{\gamma}^2/ma = 164.7 \text{ MeV} \ , \quad a^{-1} = 0.763 \text{ fm};$$

ii) the attractive plus repulsive Tabakin interaction, as parameterized by Osman[8],

$$f^{101}_{00}(k|k) = -\tilde{\gamma}^2/(k^2+a^2)^2 + \tilde{\mu}^2/(k^2+b^2)^2 \ ,$$

$$\hbar^2\tilde{\gamma}^2/ma = 160.7 \text{ MeV} \ , \ a^{-1} = 0.689 \text{ fm} \ , \tag{28}$$

$$\hbar^2\mu^2/mb = 930.5 \text{ MeV} \ , \ b^{-1} = 0.115 \text{ fm} \ ;$$

iii) the attractive-plus-repulsive oscillatory interaction of Sirohi & Srivastava[9] (which, they claim, reproduces better the repulsive parts of the better-known local potentials),

$$f^{101}_{00}(k|k) = -\frac{\tilde{\alpha}^2}{(k^2+a^2)^2}\left(\frac{\sin \mu k}{\mu k}\right)^2 + \frac{\tilde{\beta}^2 k^4}{(k^2+b^2)^2}\left(\frac{\sin \nu k}{\nu k}\right)$$

$$\tilde{\alpha} = 3.227 \text{ fm}^{-1/2} \ , \quad \tilde{\beta} = 0.736 \text{ fm}^{-1/2} \ ,$$

$$a = 1.530 \text{ fm}^{-1} \ , \quad b = 0.812 \text{ fm}^{-1} \ , \tag{29}$$

$$\mu = 0.412 \text{ fm} \ , \quad \nu = 1.385 \text{ fm} \ ;$$

iv) the purely repulsive component of the Tabakin-Osman potential (28); v) the purely repulsive component of the Sirohi & Srivastava potential (29); and vi) the purely repulsive component of the Tabakin interaction

$$f^{101}_{00}(k|k) = \tilde{\beta}^2 k^4 \left[(k-d)^2 + b^2\right]^{-2}\left[(k+d)^2 + b^2\right]^{-2} \tag{30}$$

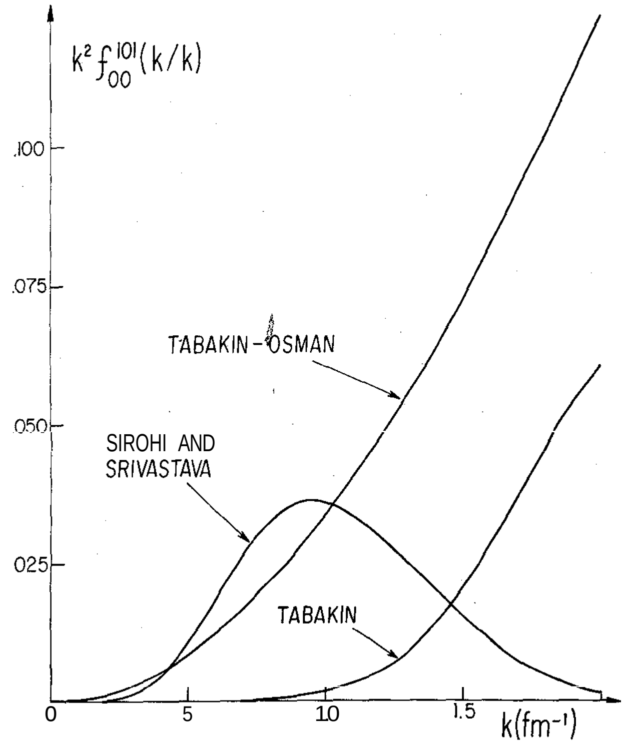

Fig.2 - Dynamic form factors $f_{00}^{101}(k|k)$ (times k^2) for the purely repulsive portion of the $^3S_1$ state non-local, separable interactions considered in Eqs. (28), (29) and (30). The energy difference Eq. (26), for k = I, would be one of these form factors times the corresponding curve in Fig.1 integrated over k from 0 to βk_F.

$$\hbar^2\tilde{\beta}^2/mb = 10.3 \text{ MeV}, b^{-1} = 0.99 \text{ fm}, \quad d^{-1} = 0.59 \text{ fm}.$$

The form factors iv) through vi) are shown in Fig.2.

4. RESULTS

The quantity $\Delta\langle v\rangle/N$ of Eq.(26) was evaluated by numerical integration. (For the simple form factors (27) to (28) a closed analytical expression can be found, cf. Appendix). This quantity was never negative for interactions i) through iii) above. For the purely repulsive iv) thrnugh vi) it could acquire negative values for some $\beta > 1$

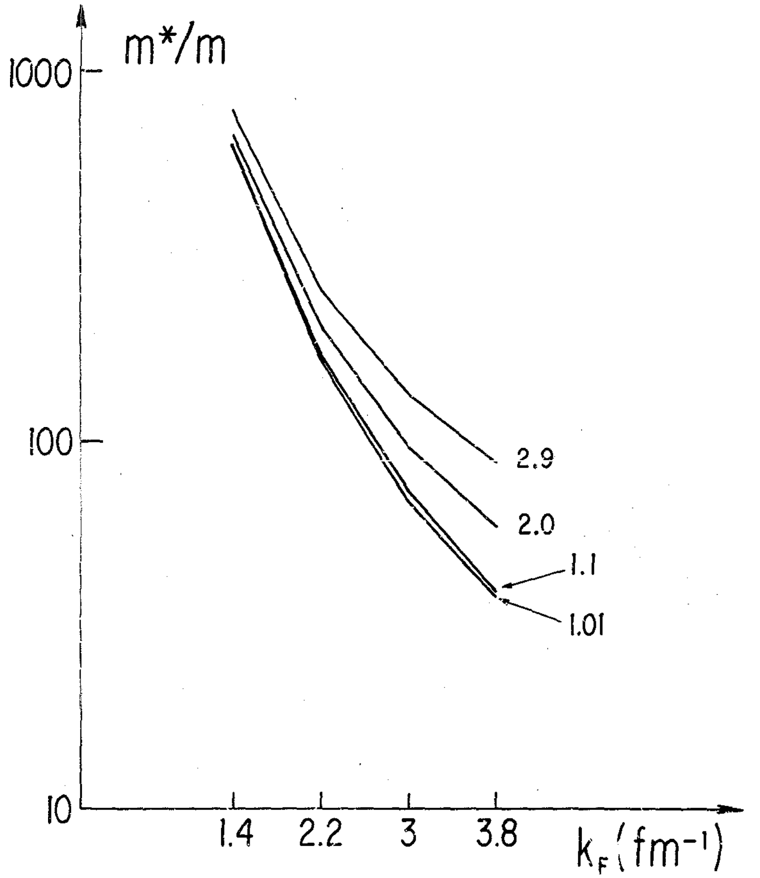

Fig.3 - Minimum value of effective mass, in units of m, the nucleon mass, m^*/m required to make the abnormally-occupied state lower in energy than the normally-occupied one, as function of k_F and for several values of $\beta>1$, for the purely repulsive part of Eq. (29).

and k_F, but never sufficiently so as to compensate for the (positive) kinetic energy difference. Making the repulsion stronger or, equivalently, increasing the particle mass by replacing m by m^*, say, would accomplish a net energy lowering of the abnormally-occupied state with respect to the normally-occupied one. In Figs 3, 4 and 5 we display the minimum values of the "effective mass" m^*, in units of the nucleon mass m required to do this for various values of $\beta>1$, for the interactions iv), v) and vi), respectively.

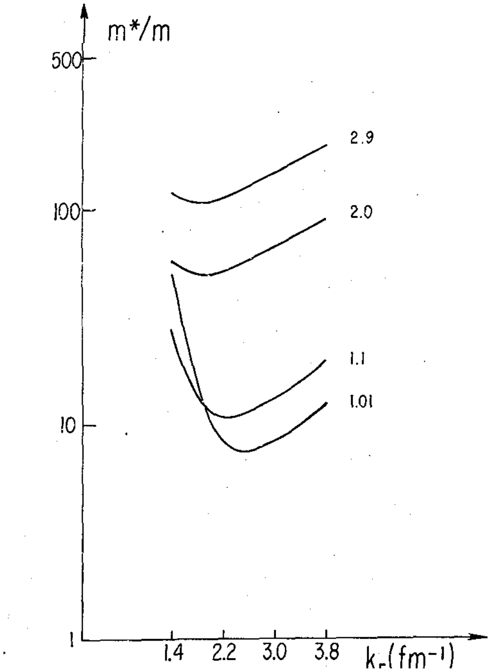

Fig.4 - Same as Fig. 3 but for the purelu repulsive part of (28).

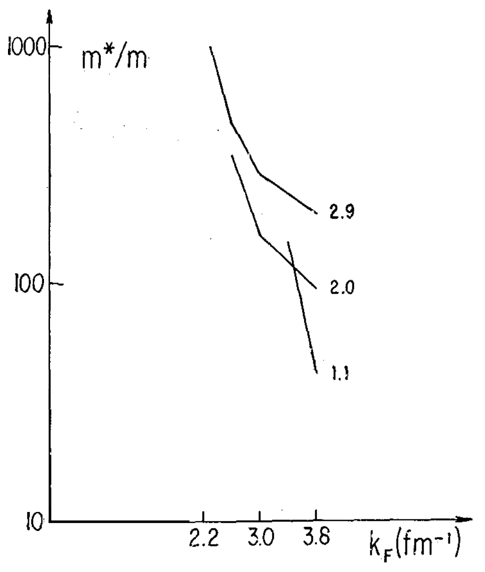

Fig.5 - Same as Fig. 3 but for the purely repulsive part of the Tabakin potential, i.e., Eq. (30).

In conclusion, we have seen that the purely repulsive parts of non-local, separable nucleon-nucleon interaction in the $^3S_1$ state, if made stronger, is sufficient to give lower energy for abnormal with respect to normal occupatíon.

APPENDIX

For dynamic form factors of the simple, but very common, type

$$f(k|k) = (k^2 + a^2)^{-2}$$

the last two integrals in (13) can both be done analytically with the results:

$$x \equiv k_F/a \quad , \quad \gamma \equiv (\beta^3-1)^{1/3} \quad ;$$

$$I(\beta;k_F) \equiv J(\beta) + J(\gamma) + L(\beta,\gamma) - \gamma^3\left[\tan^{-1}\{(\beta-\gamma)x/2\} - \frac{(\beta-\gamma)x/2}{1+(\beta-\gamma)^2x^2/4}\right];$$

$$J(\beta) \equiv \frac{1}{2}\beta^3\left\{\tan^{-1}(\beta x) + \frac{1}{\beta x} - \left[\frac{3}{2\beta x} + \frac{1}{(\beta x)^3}\right]\ell n\left[1 + (\beta x)^2\right]\right\} ,$$

$$L(\beta,\gamma) \equiv (1-2\beta^3)R_1(\beta,\gamma) + 3(\beta^2-\gamma^2)^2 x\, R_2(\beta,\gamma)/16$$

$$+ 3(\beta^2+\gamma^2)R_3(\beta,\gamma)/2x - R_4(\beta,\gamma)/x^3 \;;$$

$$R_i(\beta,\gamma) \equiv S_i([\beta+\gamma]x/2) - S_i([\beta-\gamma]x/2) \quad , \quad i = 1,2,3,4 \quad ,$$

$$S_1(y) \equiv \frac{1}{2}\left[\tan^{-1}y - y/(1 + y^2)\right] \quad ,$$

$$S_2(y) \equiv -\frac{1}{2}(1 + y^2)^{-1} \quad ,$$

$$S_3(y) \equiv \frac{1}{2}\left[\ell n(1 + y^2) + (1 + y^2)^{-1}\right]$$

$$S_4(y) \equiv \frac{1}{2}y^2(2 + y^2)(1 + y^2)^{-1} - \ell n(1 + y^2) \quad ,$$

a result which was found in agreement with the single numerical integration done before.

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