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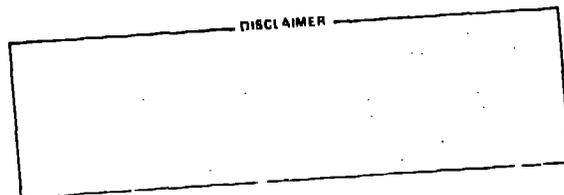
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CONF-810107--1

**TITLE: THE PERTURBATION THEORY APPROACH TO THE GROUND STATE ENERGY
IN AN INFINITE FERMION SYSTEM**

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**SUBMITTED TO: Proceedings of the Second International Conference
on Recent Progress in Many-Body Theories, Mexico City,
D.F., January 12-16, 1981**



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GROUND STATE ENERGY IN AN INFINITE FERMION SYSTEM

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ABSTRACT

The progress of the Rayleigh-Schrodinger perturbation theory approach to the computations of the ground state energy in an infinite Fermion system is reviewed.

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The fundamental question which we wish to address is, "What is an effective procedure for finding the lowest, Fermionic eigenvalue of a system described by the Hamiltonian

$$H = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i<j}^N v(|\vec{r}_i - \vec{r}_j|), \quad (1)$$

when N becomes indefinitely large?"

If V is purely repulsive, then rather good methods are available¹ over a fair range of densities and potentials, but if V is partially attractive, then the problem is much more difficult, and, of course, more interesting. There are quite a number of ways to approach the question raised above, but we will confine our discussion to perturbation methods, and their progress toward the answer to our question. In particular we will specialize in the Rayleigh-Schrödinger perturbation theory. By way of a brief review, we start with the Schrödinger equation for the Hamiltonian⁽¹⁾,

$$\left[-\frac{\hbar^2}{2m} \sum_{j=1}^N \nabla_j^2 + \sum_{i<j}^N v(r_{ij}) \right] \Psi = E\Psi, \quad (2)$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$, and we define the useful operators

$$H_0 = -\frac{\hbar^2}{2m} \sum_{j=1}^N \nabla_j^2, \quad h = \sum_{i<j}^N v(r_{ij}), \quad (3)$$

so that eq. (2) may be written more compactly as

$$(H_0 + \lambda h)\Psi = E(\lambda)\Psi. \quad (4)$$

The formulas of the Rayleigh-Schrödinger perturbation theory can then be written in terms of the energy E , and wave matrix Ω ,

$$\begin{aligned} E(\lambda) &= E_0 + E_1\lambda + E_2\lambda^2 + \dots, \\ \Omega(\lambda) &= 1 + \Omega_1\lambda + \Omega_2\lambda^2 + \dots, \\ H_0\phi &= E(0)\phi, \quad \Psi = \Omega(\lambda)\phi, \end{aligned} \quad (5)$$

and

$$E_n = \langle \phi | h \Omega_{n-1} | \phi \rangle, \quad (6)$$

$$\Omega_n = (I - P_0)(E_0 - H_0)^{-1} (h\Omega_{n-1} - \sum_{j=1}^{n-1} E_{n-j} \Omega_j),$$

where P_0 is the projection operator for the state ϕ .

The Fermi-statistics constraint is imposed by selecting the initial wave-function as a Slater determinant,

$$\phi = (N!)^{-1/2} \Gamma^{-1/2 N} \det \begin{vmatrix} \exp(i\vec{k}_1 \cdot \vec{r}_1) & \cdots & \exp(i\vec{k}_N \cdot \vec{r}_1) \\ \vdots & & \vdots \\ \exp(i\vec{k}_1 \cdot \vec{r}_N) & \cdots & \exp(i\vec{k}_N \cdot \vec{r}_N) \end{vmatrix}, \quad (7)$$

where the \vec{r}_i are the lowest N eigenstates of H_0 in a box of volume Γ with periodic boundary conditions. The corresponding momentum representation of the potential is

$$\begin{aligned} \langle \vec{v} | v | \vec{\lambda} \vec{\eta} \rangle &= \Gamma^{-2} \int_{\text{Box}} \cdots \int d^3 R d^3 r v(\mathbf{r}) \\ &\times \exp \left[i(\vec{\lambda} + \vec{\eta} - \vec{v} - \vec{\mu}) \cdot \vec{R} + \frac{1}{2} i \vec{r} \cdot (\vec{\lambda} + \vec{\eta} - \vec{v} - \vec{\mu}) \right] \\ &= (2\pi)^3 \Gamma^{-1} \delta_{\vec{\lambda} + \vec{\eta}, \vec{v} + \vec{\mu}} \tilde{v}(\frac{1}{2}(\vec{\lambda} + \vec{\eta} - \vec{v} - \vec{\mu})), \end{aligned} \quad (8)$$

where δ is Kronecker's delta and \tilde{v} is the momentum transform of $v(\mathbf{r})$. The basic formula for the graphical expansion of the Rayleigh-Schrödinger perturbation theory is

$$h\phi = \frac{1}{2} (N!)^{-1/2} \Gamma^{-1/2 N} \sum_{\vec{m}, \vec{n}} \sum_{\vec{v}, \vec{\mu}} \langle \vec{v} | v | \vec{m} \vec{n} \rangle \phi(\vec{m} \rightarrow \vec{v}; \vec{n} \rightarrow \vec{\mu}) \quad (9)$$

where \vec{m} and \vec{n} run over the indices in the Slater determinant ϕ and \vec{v} and $\vec{\mu}$ run over all momentum states. The $\phi(\vec{m} \rightarrow \vec{v})$ type notation means that $k_{\vec{v}}$ replaces $k_{\vec{m}}$ in eq. (7). This eq. expands $h\phi$ as a sum of Slater determinants.

By use of the Hugenholtz factorization theorem, we can establish the linked cluster theorem, i.e., only connected diagrams contribute to the energy. This result is important because before the work of Brueckner³, it was thought that perturbation theory was useless because every connected part contributed a factor of N so that

$$E(\lambda) = N\lambda + N^2\lambda^2 + N^3\lambda^3 + \cdots, \quad (10)$$

instead of the correct result,

$$E(\lambda) = N\lambda + N\lambda^2 + N\lambda^3 + \cdots. \quad (11)$$

There was a "physical" explanation of eq. (10). It was that for an attractive, square-well potential, there was nuclear collapse⁴ no matter how weak the attraction, so of course the perturbation theory was non-sense!

So what happened to this explanation? The answer is that the physics has not disappeared, the radius of convergence of the series (11) for $E(\lambda)/N$ is zero. Thus it need not give the results for a pure attraction while there is still the possibility that it can work for a repulsion in an asymptotic sense. It can be shown¹ that

the divergence of (11) is no worse than

$$|E_n/N| \leq M(n!)A^n, \quad (12)$$

so that the series is uniquely summable to the correct physical answer for a simple repulsive force. Thus, for at least some many-fermion, ground-state energy problems, perturbation theory can lead in principle to the correct physical answer.

There are further problems to be considered on our search for the ground state energy of a many-fermion system with attractive forces. In particular in applications like nuclear matter which are self-bound, we know that the system must be a liquid. Thus the saturation point lies on the liquid, coexistence curve in the $(k_F - \lambda)$ plane. It is reasonable on general grounds, and borne out in model calculations⁵, that the coexistence curve is a line of analytic singularities so the usual procedure of looking for a minimum is in principle only half correct. That is to say the approach from high density at fixed potential (or to weaker potential at fixed density) is fine; the part as one passes the minimum and finds increasing energy as the density is lowered further is wrong. Here we know that a two phase system occurs. The gas phase (absolute temperature in this problem is zero) is the vacuum, and the liquid is a self-bound drop. Thus the energy remains at its minimum value and does not increase. The perturbation approach, when properly used, has the advantage of approaching the saturation point along a physically correct path exclusively in the one phase region. On the contrary a purely low density rearrangement tends to pass through the two-phase region and must be viewed with great caution.

An additional problem is that of the hard-core. We know, at least for sufficiently low density, that an infinitely strong, repulsive-core potential leads to only a finite shift in energy. The classical solution to this problem in perturbation theory is to make a change of variables. For example, the function $f(r)$ defined as

$$\eta f(r) = 1 - e^{-\lambda v(r)} = \lambda v(r) - \frac{\lambda^2 v^2(r)}{2!} + \dots \quad (13)$$

has the property $\eta f(r) = 1$ for $v(r) = +\infty$, and $\eta f(r) \approx \lambda v(r)$ for small $\lambda v(r)$. Thus if we replace

$$\lambda v(r) = - \ln[1 - \eta f(r)] = \eta f(r) + \frac{1}{2} \eta^2 f^2(r) + \frac{1}{3} \eta^3 f^3(r) + \dots \quad (14)$$

in the $\lambda v(r)$ expansion we generate a new expansion in terms of $\eta f(r)$ which is not immediately singular for a repulsive hard core.

Brueckner had the idea to follow Watson's theory of multiple scattering and sum up in a K-matrix all the ladder diagrams (diagrams with only two hole-lines). These diagrams constitute all the leading order terms in a low density expansion and give good results for repulsive forces at low densities.

However, it was soon noticed by Emery⁶ that for a central repulsion with an attractive tail that no matter how weak the attraction, for a sufficiently high value of the relative angular momentum, the K-matrix equations possessed a singularity. What then is to be done about this problem? First, of course, it may be that the singu-

larity comes from Cooper pairs and that it implies that the true ground state is a "superfluid" and not a "normal" ground state. In this case the perturbation theory which we are using

$$\sum_{k=0}^{\infty} (\lim_{N \rightarrow \infty} E_k^{(N)}/N) \lambda^k \quad (15)$$

does not work. On the other hand, if such a situation does not arise physically, we need to fix our formalism to allow progress. In the context of perturbation theory several ways have been suggested. (a) Brueckner and Gammel⁷ simply modified the intermediate state denominator as

$$\frac{1}{(k'')^2 - k_0^2} \rightarrow \frac{1}{(k'')^2 - k_0^2 + \Lambda} \quad (16)$$

where even a very small Λ serves to eliminate the problem. (It also changes the answer, in principal, a little bit.) (b) Baker and Kahane⁸ solved the problem by using a different change of variables, i.e.,

$$F_{\rho}(k) = R_{\rho}(k) / \left[1 + (\frac{1}{2}\tau_1 - \tilde{a})R_{\rho}(k) \right] \quad (17)$$

where $R_{\rho}(k)$ (the "R matrix") is much better behaved. The Emery singularities now occur in $K_{\rho}(k)$ if $R_{\rho}(k) < 0$ since $\tau_1 \rightarrow \infty$ as $k \rightarrow k_F$. However, as any power of τ_1 is integrable, K can be expressed as a series expansion in R with finite coefficients. Baker and Kahane found that K itself is satisfactory for typical potentials. (c) Brandow's choice⁹ for intermediate-state energy denominators corresponds to a rearrangement of the perturbation series. It is to make the hole-line energies self-consistent in the intermediate state propagators, but to use the kinetic energy alone for the particle energies. This procedure is superficially attractive, but has a fatal flaw! Its advantages are: first, by the Hugenholtz factorization theorem the energy corrections to the hole lines, summed over all time orders, are on the energy shell and don't depend on the excitation of the Fermi sea so that they are easy to compute. Secondly, for a potential with a net attraction, there is a large energy gap at the Fermi surface, thus eliminating the Emery singularity problem. Finally, the resulting large denominators make the higher order terms smaller and thus less important. The principal disadvantage of this scheme is that it gives the *wrong* answer¹⁰! That is to say, the answer obtained in this manner using the "obvious" choice of the integration contour over intermediate state energies omits certain residue corrections which are included by the correct choice of integration contour. These details are explained at length by Baker and Gammel.¹⁰ An additional aesthetic drawback to the method is that it splits certain finite contributions into the difference of two infinite ones.

In summary then, the progress thus far by perturbation methods is: (1) The straightforward V expansion with appropriate resummations such as the K -matrix one, or the complete hole-line rearrangement with a symmetrical treatment of hole and particle energies appears to give satisfactory results for problems with purely repul-

sive forces. (2) The K-matrix and hole-line type rearrangements, as they stand, are not adequate for potentials with an attractive tail because of the Emery singularities. (3) A good change of variables, such as the R-matrix expansion⁸ would appear to allow reasonable computational progress towards our goal. Other changes of variables could profitably be explored. (4) Modern computers would appear to make much more extended work in this area possible than in the past.

This work was performed under the auspices of the U.S. D.O.E.

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