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Single-Particle Energy and Effective Mass and the Binding Energy of Many-Body Systems

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The relationship between the single-particle energy and effective mass and the binding energy of the many-particle nuclear system is discussed. It is shown that only in the case of first order perturbation theory is it possible to define a physically meaningful single-particle energy $E(p)$ so that both relationships, $E(p_F)=(p^2/2M)+V(p_F)=E_{\text{average}}$ and $NE_{\text{average}}=(p^2/2M)_{\text{average}}+\frac{1}{2}[V(p)]_{\text{average}}$, are satisfied. More generally a correction term appears, as a result of important many-body contributions to the single-particle energy which arise from the effects of the exclusion principle and from the variation of the self-consistent excitation spectrum with density. The principal effect of the correction is to alter the relationship between E_{average} and the average value of the single-particle energy. Analysis of the optical potential which determines the momentum of a nucleon interacting with the nucleus shows that the same correction term again appears, changing the usual definition of the optical potential.

An additional consequence is that it is not possible to fix the effective mass for particle motion from knowledge of the average binding energy and kinetic energy alone, the first order theory underestimating the effective mass by 38% in nuclear matter and by 77% in liquid He^3.

IN recent studies[1,2] of the properties of nuclear matter and liquid He^3,[3] a determination has been made of the energies of single-particle excitations and of the average energy per particle. In the definition of particle energies used in those calculations, it has been found that the energy of a single particle at the Fermi surface is not equal to the mean binding energy. This result is similar to an earlier result obtained by the author,[4] but does not agree with more recent discussions by Weisskopf[5] and Moszkowski.[6] It is the purpose of this note to discuss this discrepancy and to show the conditions under which the equality between the energy at the Fermi surface and the mean energy holds. The physical interpretation of the single-particle energy will also be discussed.

In the theory of the many-body system[7] used in references (1), (2), and (3), the energy of an excitation with momentum p_i is

$$E(p_i)=(p_i^2/2M)+V(p_i), \tag{1}$$

where

$$V(p_i)=\sum_j(K_{ij,\,ij}-K_{ij,\,ji}). \tag{2}$$

The sum over j runs over all filled states and includes a sum over spin and isotopic spin. The energy as defined in Eqs. (1) and (2) does not refer to an arbitrarily chosen zero point of energy. In many applications, however, it is possible to add a constant to the single-particle energy. For example, in determining the effective mass of an excitation or properties of low excited states such as the nuclear symmetry energy or the specific heat and magnetic susceptibility of He^3, only the variation of $E(p)$ with momentum enters. An arbitrary constant in the energy is meaningful, however, in determining the total energy of the system. Such a constant also affects the separation energy of a particle, since this is the difference in total energy between two systems with $N+1$ and N particles.

With the single-particle energies as defined in Eq. (1), the average energy per particle is

$$E_{\text{Av}}=\tfrac{3}{5}(p_F{}^3/2M)+V_{\text{Av}}, \tag{3}$$

where V_{Av}, the average potential energy per particle, is

$$V_{\text{Av}}=(1/2N)\sum_i V(p_i). \tag{4}$$

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[1] K. A. Brueckner and J. L. Gammel, Phys. Rev. **105**, 1679 (1957).

[2] K. A. Brueckner and J. A. Gammel, Phys. Rev. **109**, 1023 (1958).

[3] K. A. Brueckner and J. A. Gammel, Phys. Rev. **109**, 1040 (1958).

[4] K. A. Brueckner, Phys. Rev. **97**, 1353 (1955).

[5] V. F. Weisskopf, Nuclear Phys. **3**, 423 (1957).

[6] S. A. Moszkowski (private communication).

[7] A comprehensive list of references is given in reference 2.

Thus, with these definitions, the usual relationship between V_{Av} and $V(p)$ holds. This also makes it possible to use the usual physical interpretation of $V(p)$ as an energy density. We shall see in the following that if we wish to choose the zero point of energy so that the energy $E(p_F)$ of the last particle is equal to the separation energy, then it is usually necessary to depart from the definition of Eq. (2) for $V(p_i)$.

The reaction matrix K which determines the interaction energies is obtained by solving for the motion of particle pairs in the average field of the remaining particles. K is defined by the integral equation

$$K_{ij,\,kl}=v_{ij,\,kl}+\sum_{\substack{m,\,n\\ p_m\geqq p_F;\\ p_n\geqq p_F}} v_{ij,\,mn}(E_k+E_l-E_m-E_n)^{-1}K_{mn,\,kl}. \tag{5}$$

The propagator $(E_k+E_l-E_m-E_n)^{-1}$ describes the motion of the excited particles through the many-body medium. The restriction on the sum over p_m and p_n that the excited momenta be above the Fermi surface takes into account the requirements of the exclusion principle.

The reaction matrix K depends on the density explicitly through the normalization volume, since the matrix elements of V contain a factor $1/\Omega$. A further dependence of K on the density enters through the variation of p_F with the density and also through the shift with density of the self-consistent particle energy spectrum. In first approximation, K can be replaced by V and ΩV is independent of density.

Before we discuss the features of the excitation spectrum, it is convenient to summarize the interpretation of the particle excitation. We recall[8,9] that the true nuclear wave function $\psi(N)$ is related to the model or independent-particle wave function $\varphi(N)$ by the correlation function or "model operator" F, the relation being

$$\psi(N)=F\varphi(N). \tag{6}$$

To an excitation of a single particle in the model state, there corresponds a change in the state of the actual system. This change is, of course, much more complicated than the change of the model, since the correlation function F will change with excitation to take account of the change in correlation structure. The change in state of ψ upon a single-particle excitation in φ therefore must be regarded as the creation of an "exciton," i.e., a correlated change in the state of many particles which resembles a single-particle excitation only if correlation effects are neglected. It is often convenient to talk of these complex excitations by using the language of the single-particle model; it must be kept in mind, however, that the identification can be made only in the restricted sense just discussed.

In the nuclear theory, the excitons of the actual system are to be identified with the independent particles of the shell model. The energies of these particles are then $E(p)$ as given by Eq. (1). These energies are important, not only since they enter into the determination of the reaction matrix K, but also since they determine both the effective mass for particle motion and the properties of the system at low excitation.

We now return to the study of the excitation energies. We first simplify Eqs. (2) and (4) by replacing the sums by integrals, using the relation

$$\sum_i=\frac{\Omega}{(2\pi)^3}S_i\int d\mathbf{k}_i, \tag{7}$$

where by S_i we mean the sum over spin and isotopic spin. We also write

$$\frac{\Omega}{(2\pi)^3}S_iS_j(K_{ij,\,ij}-K_{ij,\,ji})=f(ij). \tag{8}$$

[As remarked above, $f(ij)$ is independent of density if K is evaluated to first order in V.] We then can rewrite Eqs. (2) and (4) as

$$V(p_i)=\tfrac{1}{4}\int d\mathbf{k}_j\, f(ij), \tag{9}$$

and

$$V_{\text{Av}}=\frac{1}{2N}\frac{\Omega}{(2\pi)^3}\int d\mathbf{k}_i\int d\mathbf{k}_j\, f(ij), \tag{10}$$

where to obtain Eq. (9) we have assumed that $V(p_i)$ has no dependence on spin or isotopic spin as is true in an unpolarized medium.

We first show that Eqs. (3) and (10) give correctly the result that the difference in the energy of $N+1$ and N particles in their ground state is equal to the mean energy per particle. To show this, it is necessary to use the fact that for the saturated system, the density and consequently the Fermi momentum p_F do not change as N is changed. Thus the energy difference is

$$E(N+1)-E(N)=\frac{3}{5}\frac{p_F^2}{2M}[(N+1)-N]+\frac{1}{2}\frac{(\Omega_{N+1}-\Omega_N)}{(2\pi)^3}\int d\mathbf{k}_i\int d\mathbf{k}_j\, f(ij). \tag{11}$$

At constant density we have $\Omega_{N+1}=[(N+1)/N]\Omega_N$, so that

$$E(N+1)-E(N)=\frac{3}{5}\frac{p_F^2}{2M}+\frac{1}{2N}\frac{\Omega_N}{(2\pi)^3}\times\int d\mathbf{k}_i\int d\mathbf{k}_j\, f(ij), \tag{12}$$

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[8] R. J. Eden and N. C. Francis, Phys. Rev. **97**, 1366 (1955); Brueckner, Eden, and Francis, Phys. Rev. **99**, 76 (1955); H. A. Bethe, Phys. Rev. **103**, 1353 (1956).

[9] The nonvanishing of Δ is due to many-body effects included in the definition of the K matrix, these arising both from the effects of the exclusion principle and from the density variation of the self-consistent excitation spectrum (see, for example, reference 2).

which is just the mean binding energy. This result of course also follows directly from the proportionality of the total energy of the system to the number of particles, i.e.,

$$E_{\text{total}}(N)=N\times E_{\text{Av}}. \tag{13}$$

We next consider the saturation condition, that E_{Av} be independent of density. This is equivalent to the requirement that $p_F(\partial E_{\text{Av}}/\partial p_F)=0$. To carry out this differentiation, we make use of the relation

$$p_F(\partial\Omega/\partial p_F)=-3\Omega, \tag{14}$$

since Ω is proportional to $1/p_F{}^3$. From Eqs. (3) and (10) we then obtain the result:

$$0=\frac{6}{5}\frac{p_F{}^2}{2M}+\frac{1}{2}\left\{-\frac{3\Omega}{(2\pi)^3N}\int d\mathbf{k}_i\int d\mathbf{k}_j\, f(ij)+\frac{2\Omega}{(2\pi)^3}\frac{4\pi k_F{}^2}{N}\int d\mathbf{k}_j\, f(ij)_{p_i=p_F}\right\}+\Delta, \tag{15}$$

where

$$\Delta=\frac{1}{2}\frac{\Omega}{(2\pi)^3N}\int d\mathbf{k}_i\int d\mathbf{k}_j\, p_F\frac{\partial f(ij)}{\partial p_F}. \tag{16}$$

This result can be simplified by use of the relation

$$4\Omega\left(\frac{4}{3}\frac{\pi k_F{}^3}{(2\pi)^3}\right)=N, \tag{17}$$

and also by using Eq. (9) for $V(p_F)$. The result is

$$0=\frac{6}{5}\frac{p_F{}^2}{2M}-\tfrac{3}{2}V_{\text{Av}}+\tfrac{3}{2}V(p_F)+\Delta. \tag{18}$$

Combining this result with Eq. (1) for $V(p_i)$, we find

$$\begin{aligned}E(p_F)&=(p_F{}^2/2M)+V(p_F)\\&=\tfrac{3}{5}(p_F{}^2/2M)+V_{\text{Av}}-\tfrac{1}{3}\Delta.\end{aligned} \tag{19}$$

Thus $E(p_F)$ is equal to $E_{\text{Av}}=\frac{3}{5}(p_F{}^2/2M)+V_{\text{Av}}$ only if Δ is equal to zero. This is true only to first order in v, as remarked above. In the actual studies of nuclear matter, the average energy per particle is -15.2 Mev while $E(p_F)$ is -27.5 Mev. In liquid He^3 the corresponding values are -0.96 and -3.61 ($k\times$degrees Kelvin) per particle. In both cases the difference is due to the last term in Eq. (19).

The discrepancy between $E(p_F)$ and E_{Av} can, of course, be removed by changing the definition of the single-particle energies. A suitable choice is

$$W(p_i)=V(p_i)+\tfrac{1}{3}\Delta, \tag{20}$$

in which case Eq. (19) leads immediately to the result

$$(p_F{}^2/2M)+W(p_F)=E_{\text{Av}}. \tag{21}$$

This redefinition leads, however, to a breakdown in the relationship between V_{Av} and $W(p_i)$, since the relation now is

$$V_{\text{Av}}=(1/2N)\textstyle\sum_i[W(p_i)-\tfrac{1}{3}\Delta]. \tag{22}$$

Consequently we cannot simultaneously maintain a simple relationship between V_{Av} and $V(p_i)$ and also the equality between $V(p_F)$ and E_{Av}.

It is interesting to see if a criterion exists to show which of the definitions given in Eq. (2) and Eq. (20) is physically more correct. The definition of $W(p_i)$ in Eq. (20) is, of course, more meaningful in that it adjusts the energy of the last particle to be equal to the separation energy. This allows a simpler meaning to be attached to the single-particle energy than if the definition of Eq. (2) is used. It is interesting, however, to see under what other circumstances $W(p_i)$ can be identified with the particle interaction energy. Consider, for example, a nucleon of energy E_1 entering a nucleus of N particles. There are two approximations to be distinguished. First, suppose that the nuclear volume does not change as the extra nucleon "1" enters. There are then two effects: the direct interaction of particle 1 with the particles N gives rise to new interaction terms, and the presence of a new particle above the surface of the Fermi gas inhibits the excited transitions of the interacting nucleons of the initial system and so changes their energy. The energy of the $(N+1)$-particle system thus is

$$\begin{aligned}E(N+1)={}&N\frac{3}{5}\frac{p_F{}^2}{2M}+\frac{p_1{}^2}{2M}+\frac{1}{2}\frac{\Omega_N}{(2\pi)^3}\int d\mathbf{k}_i\int d\mathbf{k}_j\, f(ij)_N\\&+\frac{1}{4}\int d\mathbf{k}_j\, f(ij)_N\,|_{p_i=p_1}\\&+\frac{1}{2}\frac{\Omega_N}{(2\pi)^3}\int d\mathbf{k}_i\int d\mathbf{k}_j[f(ij)_{N+1}-f(ij)_N],\end{aligned} \tag{23}$$

where $f(ij)_N$ and $f(ij)_{N+1}$ are evaluated at the original and final values of the Fermi momentum. The rise in the Fermi momentum through the addition of a particle near the Fermi surface is

$$(p_F)_{N+1}-(p_F)_N\cong(p_F)_N/3N. \tag{24}$$

Thus we can write

$$f(ij)_{N+1}-f(ij)_N\cong\frac{1}{3N}\left[p_F\frac{\partial f(ij)}{\partial p_F}\right]_N, \tag{25}$$

and

$$E(N+1)=E(N)+(p_1{}^2/2M)+V(p_1)+\tfrac{1}{3}\Delta, \tag{26}$$

where Δ is defined in Eq. (16), Since $V(p_1)+\frac{1}{3}\Delta$ is also defined to be $W(p_1)$, we simply have

$$E_1=(p_1{}^2/2M)+W(p_1). \tag{27}$$

Thus in this situation, we determine the momentum of a nucleon entering the nucleus from $W(p_1)$ and not from $V(p_1)$. This difference is in practice quite important, since $\frac{1}{3}\Delta$ is about equal to 20% of $V(p_1)$.

We consider next another possible description of the entrance of a nucleon into the nucleus. Suppose that we assume that as the extra particle is added, the nuclear volume increases so that the density remains constant. In this case, as long as the added neutron momentum is close to the Fermi surface, the reaction matrices are very weakly affected by the change in the mean Fermi momentum. The kinetic energy of the N nuclear particles drops, however, the change being

$$\frac{3}{5}\frac{p_F^2}{2M}N \rightarrow \frac{3}{5}\frac{p_F^2}{2M}N\left(\frac{\Omega_N}{\Omega_{N+1}}\right)^{\frac{2}{3}} = \frac{3}{5}\frac{p_F^2}{2M}N\left(1-\frac{2}{3N}\right). \quad (28)$$

The interaction energy of the N-particle system also changes, the drop in density being equivalent to the loss of a particle at the Fermi surface. This is partially compensated by the increase in volume, the two effects being

$$\frac{1}{2}\frac{\Omega_N}{(2\pi)^3}\int d\mathbf{k}_i\int d\mathbf{k}_j f(ij) \rightarrow -V(p_F)+(N+1)V_{\mathrm{Av}}. \quad (29)$$

Combining these results and now including the energy of the added particle with momentum p_1, we have

$$E(N+1)=E(N)+(p_1^2/2M)-\tfrac{2}{5}(p_F^2/2M) +V(p_1)-V(p_F)+V_{\mathrm{Av}}. \quad (30)$$

Using Eq. (19) for the relationship between $V(p_F)$ and V_{Av}, we find

$$E(N+1)-E(N)=E_1=(p_1^2/2M)+V(p_1)+\tfrac{1}{3}\Delta =(p_1^2/2M)+W(p_1). \quad (31)$$

Thus again we see that $W(p_1)$ determines the wave number of the added particle.

To summarize these results: We have shown that $W(p_1)$ as defined in Eq. (20) gives correctly the nuclear separation energy for $p_1=p_F$, and also is the correct single-particle or optical potential to determine the wave number of a nucleon entering a nucleus. The latter result holds in either of the two approximations of constant nuclear density or constant volume.

An additional point of interest related to the connection between $E(p_F)$ and E_{Av} occurs in the definition of the effective nucleon mass.[2,4,5] In the studies of the nuclear matter problem it has usually been possible, at least for momenta in the Fermi gas, to approximate $V(p)$ or $W(p)$ by the quadratic expansion

$$V(p)=V(0)+bp^2. \quad (32)$$

In this case, the single-particle energy is

$$E(p)=(p^2/2M^*)+V(0), \quad (33)$$

where

$$(1/M^*)=(1/M)+2b. \quad (34)$$

In this approximation the average energy per particle is

$$E_{\mathrm{Av}}=\tfrac{3}{5}(p_F^2/2M)+\tfrac{1}{2}[V(0)+\tfrac{3}{5}bp_F^2]. \quad (35)$$

By using Eqs. (33) and (34) for $V(0)$ and b and also Eq. (19) for $E(p_F)$, this can be written

$$E_{\mathrm{Av}}=\frac{3}{5}\frac{p_F^2}{2M}\left(1-\frac{2}{3}\frac{M}{M^*}\right)-\frac{1}{3}\Delta. \quad (36)$$

In the nuclear problem, $E_{\mathrm{Av}}=15.5$ Mev and the mean kinetic energy $\frac{3}{5}(p_F/2M)$ is 25.5 Mev. If Δ is set equal to zero, we then find $M^*/M=0.42$.[5] This value is considerably smaller than the computed value of 0.68 obtained in the studies of nuclear matter and also too small to reconcile with the nuclear symmetry energy.[2] The discrepancy is much more striking in the case of liquid He^3,[3] where again $E_{\mathrm{Av}}=-\frac{3}{5}[\frac{3}{5}(p_F^2/2M)]$ but $M^*/M=1.82$.

In conclusion, we wish to point out the relevance of these results to the case of the nuclear shell model. We have seen that the nature of the two-body interactions is such as to lead to large many-body corrections to the perturbation prediction of the properties of the single-particle potentials. These in particular appear in the value of approximately -12 Mev computed for the correction term $-\frac{1}{3}\Delta$ in Eq. (19). Thus, if we wish to use a single-particle model for determining the energy levels of the shell model, we must either (a) drop the assumption that the single-particle energy is to be equated to the separation energy of a nucleon or (b) drop the usual relation of Eq. (4) between binding energy and single-particle energy and replace it by a relation of the form given in Eq. (21). The latter procedure will often be the most desirable since the physical interpretation of the state of the last particle will then be the simplest. In either case the nucleon effective mass cannot be determined solely from knowledge of the average kinetic energy and average binding energy, but also requires knowledge of the nuclear "rearrangement energy" $\frac{1}{3}\Delta$.

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