Energy Level Shifts in a Large Enclosure*

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It is proved that for a particle enclosed in a large box, a potential shifts the energy levels by an amount which, as the volume v of the enclosure tends to infinity in a suitable manner, becomes proportional to $E^{\frac{1}{2}}\delta(E)v^{-\frac{1}{3}}$, where δ is the corresponding phase shift. Application of this result to the many-particle problem is discussed.

I. INTRODUCTION

IN some quantum mechanical stationary-state problems of great complexity, it is a very useful approximation to replace the part of the discrete spectrum which becomes continuous when the boundary recedes to infinity, by that continuum. In this fashion, scattering information may be used in certain bound-state problems, or else the simpler scattering formalism may be used to solve them. One needs for this purpose an understanding of the manner in which one formalism goes over into the other; more specifically, how quantities of one formalism are continuously connected with those of the other. Two such quantities of greatest physical interest are, in one case, the shift in the energy levels caused by a force, and, in the other, the scattering phase shift.

The purpose of this paper is to investigate the behavior of shifts in the energy levels of a particle in a box, due to the introduction of a potential, as the enclosure becomes infinitely large. In contrast to first appearances, it will turn out that these shifts tend to zero generally not as v^{-1}, where v is the volume of the box, but that many different limiting processes can be chosen which lead to different rates of decrease of ΔE. The limiting process of greatest physical interest yields a decrease as $v^{-\frac{1}{3}}$.

The second result of the investigation is that, with the choice of the limiting process of greatest applicability, the quantity that emerges from the energy shift of infinite volume is the phase shift itself, and not its tangent.[1] In the course of the proof of this result, the one first mentioned also emerges. It was, however, found instructive to investigate the first separately.

In Sec. II we show that with an appropriately chosen way of letting the volume tend to infinity, the energy shift tends to zero as $v^{-\frac{1}{3}}$. In Sec. III we discuss the effect of this result on a recent paper[2] which purported to show that the large-volume limit of the relevant bound-state integral equation is that of the K matrix.

In Sec. IV we prove that for a central potential

$$\lim_{v\to\infty} v^{\frac{1}{3}}\Delta E(E) = -2Ek^{-1}\delta_l(E).$$

This equation is then generalized to the inclusion of a tensor force.

In Sec. V, finally, we discuss the applicability of the result of Sec. IV to cases of physical interest, such as many-body interactions and, specifically, the "coherent model" of the nucleus.

II. DERIVATION OF $\Delta E \sim v^{-\frac{1}{3}}$

We consider a single particle confined to the interior of a box. Each energy level E_{0n} allowed in the absence of forces other than the walls, will be shifted to a new value $E_n = E_{0n} + \Delta E(E_{0n})$ in the presence of a potential. Being interested in only those levels E_n which do not remain a part of the discrete spectrum as the box becomes infinitely large, we are going to investigate the question: How fast does ΔE tend to zero as the walls of the enclosure recede to infinity?

The Schrödinger equation in the absence of forces is

$$(H_0 - E_{0n})\psi_{0n} = 0, \quad (1)$$

and the boundary condition demands that ψ_{0n} be zero on the walls of the box.[3] In the presence of the potential V, the Schrödinger equation becomes

$$(H_0 + V - E_n)\psi_n = 0, \quad (2)$$

while the boundary condition remains unchanged.

Taking the inner product of (2) with ψ_{0n} on the left and using (1), we obtain

$$(\psi_{0n}, V\psi_n) - \Delta E(E_{0n})(\psi_{0n}, \psi_n) = (H_0\psi_{0n}, \psi_n) - (\psi_{0n}, H_0\psi_n). \quad (3)$$

By virtue of the boundary condition obeyed by both ψ_{0n} and ψ_n, the right-hand side of (3) vanishes and we get the well-known result

$$\Delta E(E_{0n})(\psi_{0n}, \psi_n) = (\psi_{0n}, V\psi_n). \quad (4)$$

The purpose of the rederivation was but to recall that (4) depends on the fact that both ψ_{0n} and ψ_n satisfy the boundary condition.

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[1] These points were also mentioned in a somewhat different connection in a letter by N. Fukuda, Progr. Theoret. Phys. (Japan) (to be published).

[2] Reifman, DeWitt, and Newton, Phys. Rev. **101**, 877 (1956).

[3] Any other boundary condition, e.g., that the normal derivative of the wave function vanish, or a mixed one, or a periodic one, would serve as well. We are adopting the one mentioned merely for the sake of definiteness.

We now consider the case of a central potential and choose the enclosure to be spherical, of radius R. Because the potential is spherically symmetric, both E_{0n} and E_n are associated with a single[4] angular momentum l. There are, then, $2l+1$ linearly independent unnormalized free wave functions of the form

$$\psi_{0n}(\mathbf{r})=j_l(k_{0n}r)Y_l(\theta,\varphi), \qquad (5)$$

where j_l is a spherical Bessel function, and Y_l is a surface harmonic. They satisfy the boundary condition by virtue of the equations

$$Rk_{0n}=a_n{}^l, \quad j_l(a_n{}^l)=0, \qquad (6)$$

from which E_{0n} is obtained as

$$E_{0n}=(\hbar^2/2m)k_{0n}{}^2=(\hbar/2m)(a_n{}^l/R)^2.$$

Let us assume that the potential V is sufficiently well behaved so that its first and second absolute moments exist:

$$\int_0^\infty dr\, r|V(r)|<\infty, \quad \int_0^\infty dr\, r^2|V(r)|<\infty.$$

Then the "perturbed"[5] wave function corresponding to (5) is

$$\psi_n(\mathbf{r})=(k_nr)^{-1}\varphi_l(k_n,r)Y_l(\theta,\varphi), \qquad (7)$$

where φ_l is a regular radial wave function[6] that satisfies the same boundary condition at the origin as does $krj_l(kr)$:

$$\lim_{r\to 0}[\varphi_l(k,r)/krj_l(kr)]=1.$$

Consequently, in the coordinate representation

$$(\psi_{0n},\psi_n)=\int d\Omega\int_0^R dr\, r^2 j_l(k_{0n}r)(k_nr)^{-1} \times\varphi_l(k_n,r)Y_l{}^*(\theta,\varphi)Y_l(\theta,\varphi)$$
$$=ck_n{}^{-1}\int_0^R dr\, rj_l(k_{0n}r)\varphi_l(k_n,r). \qquad (8)$$

The numbers k_{0n} and l being freely selected first and $R=R_0$ subsequently chosen so that $R_0k_{0n}=a_n{}^l$ for some n, we now let R take on increasing values of the sequence

$$R_i=a_{n+i}{}^l/k_{0n}, \quad \cdots<R_i<R_{i+1}<\cdots. \qquad (9)$$

By k_n we mean that perturbed level which goes over continuously into k_{0n} if the potential vanishes while R is fixed.[2] Then

$$k_n\to k_{0n}, \quad \text{as} \quad R\to\infty.$$

The asymptotic behavior of (8) for large R is now simple to establish. Since $krj_l(kr)$ and $\varphi_l(k,r)$ both are asymptotic to sine waves, the right-hand side goes to infinity as R. Regardless of the detailed approach of k_n to k_{0n}, we need only avail ourselves of the boundedness[7] of both $krj_l(kr)$ and $\varphi_l(k,r)$ as a function of r and k on the real line to see that

$$|(\psi_{0n},\psi_n)|\leqslant AR,$$

where A is a constant depending on k_{0n}, l, and the potential.

The right-hand side of (4) is bounded and, if ψ_{0n} and ψ_n are not normalized, it will usually not tend to zero as R tends to infinity. The quantity

$$\lim_{R\to\infty}(\psi_{0n},V\psi_n)=ck_{0n}{}^{-1}\int_0^\infty dr\, rj_l(k_{0n}r)\varphi_l(k_{0n},r)V(r)$$

is finite and generally different from zero. It follows that in general

$$\lim_{R\to\infty}\Delta E(E_{0n})R\neq 0, \qquad (10)$$

or $\Delta E\sim R^{-1}$. The numerical value of the limit in (10) will be obtained in Sec. IV.

The sequence (9) of box sizes is, of course, not the only one possible. Its peculiarity is that there is always a level of the same angular momentum l at $k=k_{0n}$. One could, alternatively, take a sequence R_i' so that the next level, regardless of the angular momentum, always comes to lie on k_{0n} and no levels are left out. Since, however, R_i' is a subsequence of R_i', either $\lim(R_i\Delta E)=\lim(R_i\Delta E)$, or else that limit does not exist at all.

One could, nevertheless, choose a different subsequence of R_i', in which $l\to\infty$ and $\lim(R\Delta E)=0$. There exists in this manner, indeed, a wide variety of choices with correspondingly different rates of decrease of ΔE. None of these seem to us to be of any particular physical interest.

The same result as (10) is obtained in the first approximation for a weak potential. Then (4) becomes

$$\Delta E(\psi_{0n},\psi_{0n})=(\psi_{0n},V\psi_{0n}). \qquad (4a)$$

If ψ_{0n} is normalized to unity, then this is, of course, simply the first term in the perturbation expansion

$$\Delta E(E_{0n})=V_{nn}+\sum_{k\neq n}\frac{V_{nk}V_{kn}}{E_{0n}-E_{0k}}+\cdots. \qquad (4b)$$

The approach from (4) serves as a reminder that ψ_{0n}, that is, the states between which the matrix elements V_{nk} are taken, must satisfy the boundary condition. In the case of a spherical boundary, they must therefore be of the form (5) and hence carry a normalization factor which vanishes as $R^{-\frac{1}{2}}$ for large R.

It is instructive to consider also the situation in which the boundary has the form of a cube rather than a sphere. The unperturbed wave functions are then

[4] Except in the case of accidental degeneracy, which would depend on the potential and on R. We may safely disregard this possibility.

[5] Although we are not going to use perturbation theory, we shall conveniently employ its language.

[6] See R. Jost, Helv. Phys. Acta **20**, 256 (1947); also N. Levinson, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. **25**, No. 9 (1949).

[7] See N. Levinson reference 6; also, R. G. Newton and R. Jost, Nuovo cimento **1**, 590 (1955).

plane waves, whose normalization factors are, of course, $v^{-\frac{1}{2}}$. There is, however, a degeneracy; and it is a well-known result of degenerate perturbation theory that (4a), or (4b), is applicable only if ψ_{0n} are the "proper linear combinations" for which V has no off-diagonal matrix elements coupling state of equal energy. Simple plane waves are not such proper linear combinations.

If the plane-wave solutions that satisfy the boundary condition are

$$\exp(i\mathbf{k}_n{}^{(\alpha)}\cdot\mathbf{r}),\ \alpha=1,\ \cdots,N,\ \mathbf{k}_n{}^{(\alpha)2}=2mE_n/\hbar^2,$$

where N is the degeneracy, then the proper unperturbed wave functions for the perturbation theory are of the form

$$\psi_{0n}{}^{(i)}(\mathbf{r})=\sum_{\alpha=1}^{N}a_\alpha{}^{(n,i)}\exp(i\mathbf{k}_n{}^{(\alpha)}\cdot\mathbf{r}),$$

so that

$$\int(d\mathbf{r})\psi_{0n}{}^{(i)*}(\mathbf{r})V(r)\psi_{0n}{}^{(j)}(\mathbf{r})=0,\quad i\neq j.$$

Now, the normalization integral

$$\int_{\text{cube}}(d\mathbf{r})\psi_{0n}{}^{(i)*}(\mathbf{r})\psi_{0n}{}^{(i)}(\mathbf{r})=\sum_\alpha|a_\alpha{}^{(n,i)}|^2\int_{\text{cube}}(d\mathbf{r})+\sum_{\alpha\neq\beta}a_\alpha{}^{(n,i)}a_\beta{}^{(n,i)*}\times\int_{\text{cube}}(d\mathbf{r})\exp[i(\mathbf{k}_n{}^{(\alpha)}-\mathbf{k}_n{}^{(\beta)})\cdot\mathbf{r}].\quad(11)$$

The integral in the first term on the right-hand side is v, while that in the second increases as $v^{\frac{2}{3}}$ for large v. We must examine how large the degeneracy N is.

Since the number of states per unit length in k space increases as L, if L is the side length of the cube, the number of states per unit area, in some appropriate sense, goes up as L^2. Hence as L increases, the maximum number of states on a spherical surface in k space will increase as L^2. That is to say, there will certainly exist an unbounded monotonic sequence L_i and a constant c so that, whenever $L=L_i$, $N\geqslant cL^2$. That is the kind of sequence we shall choose.[8] It is proved in the first appendix that this corresponds to a choice similar to that of keeping l constant in the spherical case.

It must be recognized, however, that other choices are possible. In particular, it may be possible to pick such a sequence L_i that there never is any degeneracy at all when $L=L_i$. In that case, of course, nondegenerate perturbation theory is applicable and $\Delta E\sim v^{-1}$. Consequently we note that, by itself, the question of how rapidly ΔE tends to zero for a large enclosure is ill defined; it becomes well defined only by choice of a limiting process. In the event the box is a cube, the preferred choice is not obvious, as it is in the spherical case.

Since with our choice of limiting process the degeneracy N increases as $v^{\frac{2}{3}}$ for large v, the number of terms in the first sum on the right-hand side of (11) increases as $v^{\frac{2}{3}}$ and that in the second, as $v^{4/3}$. In general, almost all of the numbers $a_\alpha{}^{(n,i)}$ will be different from zero (see Appendix A) and since we mean them to be entirely unnormalized, dependent only on the direction $\mathbf{k}_n{}^{(\alpha)}$, they will not tend to zero as $v\rightarrow\infty$. The total increase of both terms on the right-hand side of (11) is therefore as $v^{5/3}$. (Hence, if $\psi_{0n}{}^{(i)}$ is to be normalized, the normalization factor vanishes as $v^{-5/6}$ for large v; $v^{-\frac{2}{3}}$ of that dependence is more naturally associated directly with the $a_\alpha{}^{(n,i)}$. There remains then, as in the spherical case, an "outside" factor of $v^{-1/6}$.)

The right-hand side of (4a), on the other hand, is

$$\int(d\mathbf{r})\psi_{0n}{}^{(i)*}(\mathbf{r})V(r)\psi_{0n}{}^{(i)}(\mathbf{r})=\sum_\alpha|a_\alpha{}^{(n,i)}|^2\int_{\text{cube}}(d\mathbf{r})V(r)+\sum_{\alpha\neq\beta}a_\alpha{}^{(n,i)}a_\beta{}^{(n,i)*}\times\int_{\text{cube}}(d\mathbf{r})V(r)\exp[i(\mathbf{k}_n{}^{(\alpha)}-\mathbf{k}_n{}^{(\beta)})\cdot\mathbf{r}].$$

Here the first term increases as $v^{\frac{2}{3}}$, the second as $v^{4/3}$. It follows that ΔE vanishes for large volumes as $v^{4/3-5/3}=v^{-\frac{1}{3}}$, as for a spherical box.[9]

III. EFFECT OF $\Delta E\sim v^{-\frac{1}{3}}$ ON A BOUNDARY CONDITION

In the past it has been a common misapprehension that generally $\Delta E\sim v^{-1}$, a result obtained very simply from (4a) by inserting for ψ_{0n} a plane wave. The latest victims of this error were the authors (among them one of the present authors, R.G.N.) of a recent note[2] which purported to demonstrate the limiting process from the bound-state situation to that of scattering.

In reference 2 the integral equation satisfied by an operator R_b was considered such that

$$V\psi_n=R_b(E_n)\psi_{0n}.\quad(12)$$

It was then shown that as $R\rightarrow\infty$ according to a process such as (9), the integral equation satisfied by $R_b(E_{0n})$ goes over into that for the K matrix, containing the Cauchy principal value of the integral. For the energy shift, however, one requires $R_b(E_n)$:

$$\Delta E=(\psi_{0n},R_b(E_n)\psi_{0n}),\quad(13)$$

[8] It is also relevant to count the number of states in a fixed spherical shell whose thickness decreases as L^{-1}, rather than the exact degeneracy. That takes into account also those states which approach the given level more rapidly than L^{-1} and therefore cross the perturbed level. The number of these states too increases as L^2.

[9] In the case of a parallelepiped boundary, there may be much less degeneracy. As in the case of the cube, however, levels coalesce in groups more rapidly than $v^{-\frac{1}{3}}$, while the spacing between different groups decreases as $v^{-\frac{1}{3}}$. Ordinary perturbation theory is therefore again inapplicable because many levels, whose number increases as $v^{\frac{2}{3}}$, cross the perturbed one. One handles that situation most easily by considering each such group as one degenerate level, in which case the reasoning is the same as in the case of the cube.

with appropriate normalization. Now since both $E_n - E_{0n}$ and $E_{0\ n+1} - E_{0\ n-1}$ tend to zero as R^{-1}, the shifted level E_n will not, in the limit, be symmetric between $E_{0\ n-1}$ and $E_{0\ n+1}$, as is E_{0n}. Hence it follows by the same argument which leads to K in the case of $R_b(E_{0n})$, that the limiting integral equation for $R_b(E_n)$ contains a boundary condition different from that expressed by the principal value.

The precise nature of the correct boundary condition for $R_b(E_n)$ depends both on the potential and on the energy, because the asymmetry of E_n between $E_{0\ n-1}$ and $E_{0\ n+1}$ does. Since, as we shall see below, the latter is a function of the phase shift, knowledge of the boundary condition presupposes knowledge of the solution.[10] A rather complicated self-consistency requirement is thereby introduced.

IV. CONNECTION WITH THE PHASE SHIFT

The next question is that of the actual value of $\lim(R\Delta E)$ as $R\to\infty$. We obtain this quantity as follows[11]: Let the energy level $E_n = (\hbar^2/2m)k_n^2$ be associated with the angular momentum l. Then the unnormalized wave functions are of the form (7), where

$$\varphi_l(k,r) \propto f_l(k,r) - (-1)^l \exp[2i\delta_l(k)] f_l(-k,r). \quad (14)$$

Here $f_l(k,r)$ is a solution of the lth angular momentum radial Schrödinger equation that satisfies the boundary condition[6]

$$\lim_{r\to\infty} \exp[i(kr - \tfrac{1}{2}\pi l)] f_l(k,r) = 1. \quad (15)$$

The function $\exp(2i\delta_l)$ is the lth eigenvalue of the S matrix, δ_l being the phase shift due to the potential V.

The number k_n is obtained by solving the equation

$$\varphi_l(k_n,R) = 0$$

or

$$(-1)^l f_l(k_n,R)/f_l(-k_n,R) = \exp[2i\delta_l(k_n)]. \quad (16)$$

The corresponding equation in the absence of a potential is

$$(-1)^l f_{0l}(k_{0n},R)/f_{0l}(-k_{0n},R) = 1. \quad (17)$$

In order to associate the level k_n with a specific unperturbed level k_{0n}, we divide (16) by (17) and then let R increase to infinity via (9). We obtain, by the boundary condition (15),

$$\lim_{R\to\infty} \exp[-2i(k_n - k_{0n})R] = \exp[2i\delta_l(k_{0n})], \quad (18)$$

and hence

$$\lim_{R\to\infty} (k_n - k_{0n})R = -\delta_l(k_{0n}), \quad (19)$$

or

$$\lim_{R\to\infty} \Delta E(E)R = -(2E/k)\delta_l(E). \quad (20)$$

The above procedure can readily be generalized to the case in which the potential includes that of a tensor and spin-orbit force. In that event we consider (2×2)-matrix radial wave functions of the kind used by Newton.[12]

The unnormalized radial bound-state wave function is of the form $M\Phi_l(k_n,r)$, where M is a matrix and

$$\Phi_l(k_n,r) = F_l(k_n,r) - (-1)^l S_l(k_n) F_l(-k_n,r), \quad (21)$$

if the bound state is one of a mixture of angular momenta l and $l+2$. Here $F_l(k,r)$ is a (2×2)-matrix solution of the coupled radial Schrödinger equations for angular momenta l and $l+2$ which satisfies the boundary condition

$$\lim_{r\to\infty} \exp[i(kr - \tfrac{1}{2}\pi l)] F_l(k,r) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (22)$$

$S_l(k)$ in (21) is the S matrix for angular momenta l and $l+2$. It can be written

$$S_l(k) = W^{-1}(k) s(k) W(k), \quad (23)$$

where

$$s(k) = \begin{pmatrix} \exp[2i\delta_\alpha(k)] & 0 \\ 0 & \exp[2i\delta_\beta(k)] \end{pmatrix}, \quad (24)$$

and

$$W(k) = \begin{pmatrix} \cos\epsilon(k) & -\sin\epsilon(k) \\ \sin\epsilon(k) & \cos\epsilon(k) \end{pmatrix}. \quad (25)$$

The values k_n are obtained by setting

$$\det\Phi_l(k_n,R) = 0. \quad (26)$$

This equation determines not only k_n but also a Hermitian projection $P(k_n)$ such that

$$P(k_n)\Phi_l(k_n,R) = 0. \quad (27)$$

This projection is a measure of the mixture of angular momenta in the bound state with binding energy $E_n = (\hbar^2/2m)k_n^2$.

In the absence of a potential, we have

$$S_l(k) = \mathbf{1}$$

and

$$P(k_{0n})\Phi_{0l}(k_{0n},R) = 0, \quad (28)$$

where either

$$P(k_{0n}) = P_0 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

or

$$P(k_{0n}) = \mathbf{1} - P_0 \equiv \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

In the first instance, the "unperturbed" bound state is one of angular momentum l, in the second, of $l+2$. It

[10] For the correct boundary condition, see B. S. DeWitt, Phys. Rev. **103**, 1565 (1956), following paper. See also, K. M. Watson and W. B. Riesenfeld (to be published).

[11] An argument similar to the one used here appears in the work of E. Beth and G. E. Uhlenbeck, Physica **3**, 727 (1936); **4**, 915 (1937); L. Gropper, Phys. Rev. **50**, 963 (1936); see also D. ter Haar, *Elements of Statistical Mechanics* (Rinehart Publishing Company, New York, 1954), p. 196. The use made of it there, however, and its purpose were somewhat different.

[12] R. G. Newton, Phys. Rev. **100**, 412 (1955).

must then be possible to write

$$P(k_n)=U^{-1}(k_n)P(k_{0n})U(k_n), \qquad (29)$$

where U is unitary and $\det U=+1$. This expresses merely the requirement that the bound state at k_n be continuously connected with the unperturbed state at k_{0n}. If that were not so, the energy shift ΔE would not be a well defined quantity.

We now multiply (27) by $U(k_n)$ on the left, by $F_l^{-1}(-k_n,R)W^{-1}(k_n)$ on the right, and use (21), (23), and (28). The result is

$$\begin{aligned}P(k_{0n})F_l(-k_{0n},R)F_l^{-1}(k_{0n},R)\\ \times U(k_n)F_l(k_n,R)F_l^{-1}(-k_n,R)W^{-1}(k_n)\\ =P(k_{0n})U(k_n)W^{-1}(k_n)s(k_n).\end{aligned} \qquad (30)$$

At this point, R is allowed to increase to infinity via (9). Because of (22), we obtain.

$$\begin{aligned}P(k_{0n})U(k_{0n})W^{-1}(k_{0n})\lim \exp[-2i(k_n-k_{0n})R]\\ =P(k_{0n})U(k_{0n})W^{-1}(k_{0n})s(k_{0n}).\end{aligned}$$

It follows from this that

$$\lim_{R\to\infty} U(k_n)=W(k_{0n}), \qquad (31)$$

and

$$\lim_{R\to\infty}(k_n-k_{0n})R=\begin{cases}-\delta_\alpha(k_{0n}), & \text{if } P(k_{0n})=P_0,\\ -\delta_\beta(k_{0n}), & \text{if } P(k_{0n})=1-P_0.\end{cases} \qquad (32)$$

We therefore again obtain an equation of the form (19), with the first eigen phase shift appearing if the level was shifted from one of angular momentum l, and with the second eigen phase shift if it was shifted from one of angular momentum $l+2$. (These two alternatives have, of course, nothing to do with the question of which of the two angular momenta predominates, in any sense, in the bound state.)

V. DISCUSSION AND APPLICATION

The question arises, under what conditions it is a good approximation to replace ΔE by $-2Ek^{-1}\delta_l(E)R^{-1}$, or equivalently, the bound-state equation containing a sum over discrete states, by an integral equation with the appropriate boundary condition. Since (19) was obtained by replacing, at the boundary, the spherical Bessel functions by their asymptotic values, the criterion of validity is that

$$kR\gg l\equiv kR_1. \qquad (33)$$

Classically speaking, this means that we are excluding a situation in which the particle spends all of its time in a shell extending from R to an inner radius R_1 comparable with R. Only those particles will fail to "see" the boundary which spend a much larger amount of time near the center than in any equal volume relatively close to the periphery.[13]

[13] This last formulation must be taken with a grain of salt, because it alone might lead one to suppose that only a relatively thin shell is excluded, $(R-R_1)/R\ll 1$. But that is a much weaker restriction than (33).

In many problems of physical interest, the situation is not that of a single particle with a fixed central potential, but that of two particles with an interaction. Now, since neglect of the boundary restricts us to particles "near the center" (in the above sense) anyway, for these particles the problem of "interaction plus walls" should be approximately replaceable by that of "fixed potential plus wall." In other words, if both particles tend to be near the center of a well, then the two individual wells they see are not very different and hence are approximately replaceable by one well for the center-of-mass coordinates and one well for the relative coordinates. In that case the results of this paper are applicable.

We now wish to apply our results to a problem of many particles with short-range interactions. The first simplification to be introduced is the replacement of the complicated potential that an individual particle sees, by an average constant one, depending on its energy. To the extent to which we neglect interactions involving more than two bodies, we can take for this potential the sum of the energy shifts experienced by the particle due to its interaction with all other particles, one at a time

$$V(k)=\sum \Delta E. \qquad (34)$$

The calculation of $V(k)$ by (34) is now a matter of solving a number of two-body problems. One must, then, take two particles at a time and calculate the energy shift caused by the interaction between them. The sum of these energy shifts is

$$V(k_1)=\sum_{k,l}\Delta E_l(k)N(k,l|k_1),$$

where $N(kl|k_1)$ is the average number of particles with relative momentum k and relative angular momentum l when "colliding" with particle No. 1, which has momentum k_1. When the enclosure is large, we use (20):

$$V(k_1)=-\int dk2Ek^{-1}\sum_l \delta_l(k)N(k,l|k_1)R^{-1}. \qquad (35)$$

If the number of particles is proportional to the volume, then the number $N(k,l|k_1)$ must increase linearly with R in order for

$$\sum_{l=0} N(k,l|k_1)$$

to increase as R^3, since N increases linearly with l. Consequently, $V(k_1)$ becomes independent of R.

We may apply (35) to the case of a nucleus, and compare the result with Brueckner's. It is shown in the second appendix that if we neglect surface effects, then

$$N(k,l|k_1)=4\pi^{-1}R(2l+1)g(k,k_1), \qquad (36)$$

where

$$g(k,k_1)=1+\mu(k,k_1), \qquad (37)$$

$$\mu(k,k_1)=\text{lesser of}\left[1,\frac{k_F^2-k_1^2-4k^2}{4kk_1}\right]. \qquad (38)$$

The function $g(k,k_1)$ is the (unnormalized) probability for encountering the relative momentum k if the momentum of particle No. 1 is k_1. It is the same as the function $P(k',k)$ used by Brueckner.[14] Use of (36) in (35) then leads to

$$V(k_1)=-\frac{8\hbar^2}{\pi M}\int_0^{\frac{1}{2}(k_1+k_F)} f_1(k)g(k,k_1)k^2dk, \quad (39)$$

where[15]

$$f_1(k)=k^{-1}\sum_l (2l+1)\delta_l(k). \quad (40)$$

If spin and isotopic spin are taken into account, then $f_1(k)$ must be replaced by

$$\tfrac{1}{4}f(k)=\tfrac{1}{4}(f_{ss}+3f_{ts}+3f_{st}+9f_{tt}),$$

whereupon (39) becomes

$$V(k_1)=-\frac{2\hbar^2}{\pi M}\int_0^{\frac{1}{2}(k_1+k_F)} f(k)g(k,k_1)k^2dk. \quad (41)$$

Equation (41) is now in precisely the same form as Brueckner's.[16] The only difference is the occurrence of $\delta_l(k)$ in (40), compared to Brueckner's use of $\tan\delta_l(k)$.[17]

The self-consistent approach used in the recent formulation of the "coherent model"[18] of the nucleus and described in terms of energy shifts in reference 2, is equally applicable to (39). In that case, δ_l would be calculated in the presence of $V(k)$.

The use of (20) for a many-particle system has been subjected to a check in statistical mechanics,[19] where it can be applied to the calculation of the second virial coefficient. The result agrees with that of Beth and Uhlenbeck.[11] The use of Brueckner's result does not lead to a similar agreement.

As far as the applicability of (41) to nuclear physics is concerned, a word of caution is necessary. While we believe that the arguments of this paper tend to render Brueckner's use of $\tan\delta$ (and, equivalently, of the principal value in his integral equation), in a situation where both his and our approaches are applicable, extremely dubious, there is another effect which neither his nor our result fully take into account: the exclusion principle.[20] In a high-density fermion system, the use of an ordinary "free" scattering phase shift is of course unjustified. On the other hand, if the exclusion principle is to be taken into account in some approximate manner by suitably modifying the phase shifts used, then δ no longer has the significance of a phase shift and it becomes a matter merely of notation whether the quantities used are called $\tan\delta$ or δ. The modifications due to the full use of the exclusion principle are at present unknown.

[14] K. A. Brueckner, Phys. Rev. **96**, 508 (1954), Eq. (22). This equation, however, contains an error. The factor multiplying the square bracket should be (k_0/kk') instead of (k_0/k). Brueckner's k is our k_1, and his k' is our k. Neglect of surface terms means setting $k_0=0$. Then Brueckner's (22) reduces to our (37).

[15] The fact that in (39) we have used (20) even in the case of large relative angular momenta l is of no importance, because then δ_l is small anyhow. In practice one will use only the first terms of (39).

[16] Reference 14, Eq. (21). The minus sign is there incorporated in $f(k)$. There is a factor of k'^2 missing in the integrand of (21).

[17] Brueckner, Levinson, and Mahmoud, Phys. Rev. **95**, 217 (1954), Eq. (30).

[18] K. A. Brueckner, Phys. Rev. **97**, 1353 (1955); K. A. Brueckner and C. A. Levinson, Phys. Rev. **97**, 1344 (1955); R. J. Eden and C. N. Francis, Phys. Rev. **97**, 1366 (1955); Brueckner, Eden, and Francis, Phys. Rev. **98**, 1445 (1955); **99**, 76 (1955); **100**, 891 (1955).

[19] We are indebted to Professor K. M. Watson, who carried out this check.[10]

[20] We gratefully acknowledge an interesting discussion on this point with Professor K. A. Brueckner.

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APPENDIX A

We want to show here that the number of nonvanishing coefficients $a_\alpha^{(n,i)}$ in the proper linear combinations of plane waves for perturbation theory increases as $v^{\frac{2}{3}}$.

We can write

$$\psi_{0n}^{(i)}(\mathbf{r})=\sum_{\alpha=1}^{N} a_\alpha^{(n,i)}\exp(i\mathbf{k}_n^{(\alpha)}\cdot\mathbf{r}) =\sum_{l,m} b_{lm}^{(n,i)} j_l(k_nr)Y_l^m(\mathbf{r}).$$

As the volume increases to infinity, the functions $j_l(k_nr)Y_l^m(\mathbf{r})$ satisfy the boundary condition better and better. Since, moreover, $V_{lm,l'm'}$ is diagonal, each ψ_{0n}, if the limiting process is properly chosen, will for large v approach a multiple of a single

$$4\pi j_l(k_nr)Y_l(\mathbf{r})=i^{-l}\int d\Omega_k \exp(i\mathbf{k}_n\cdot\mathbf{r})Y_l(\mathbf{k}),$$

where Y_l is some surface harmonic.

For large v, by standard arguments,

$$\sum_\alpha \rightarrow \int d\Omega_k k^2(L/\pi)^2,$$

and hence

$$\sum_\alpha a_\alpha^{(n,i)}\exp(i\mathbf{k}_n^{(\alpha)}\cdot\mathbf{r})\rightarrow (L/\pi)^2\int d\Omega_k k_n^2 a^{(n,i)}(\mathbf{k}_n)\exp(i\mathbf{k}_n\cdot\mathbf{r}) =c\int d\Omega_k Y_l(\mathbf{k}_n)\exp(i\mathbf{k}_n\cdot\mathbf{r}).$$

Comparison shows that for large v

$$a_\alpha^{(n,i)} \propto Y_l(\mathbf{k}_n)$$

for some l. The fixed number of zeros of the right hand side can make only a limited number of a_α's vanish. Hence the number of nonzero a_α's must still increase as L^2.

The argument presented shows the connection between the large degeneracy and the limiting process with constant l used in a spherical box. A sequence of box sizes which keeps the growth of degeneracy to less than L^2 corresponds to one in the spherical case in which l is allowed to increase to infinity.

APPENDIX B

The probability that if particles number 1 and 2 have momenta and angular momenta k_1, l_1, m_1, and k_2, l_2, m_2, the relative momentum and angular momentum measured are k, l, m, is given by

$$P(klm|k_1l_1m_1k_2l_2m_2) = \int (d\mathbf{k}')(d\mathbf{k}_1')(d\mathbf{k}_2')P(klm|\mathbf{k}')P(\mathbf{k}'|\mathbf{k}_1'\mathbf{k}_2') \times P(\mathbf{k}_1'|k_1l_1m_1)P(\mathbf{k}_2'|k_2l_2m_2), \quad \text{(B.1)}$$

in a self-explanatory notation.

The probability $P(klm|\mathbf{k}')$ is readily obtained from the well-known expansion

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{lm} i^l Y_l^m(\mathbf{k})^* Y_l^m(\mathbf{r}) j_l(kr).$$

The normalized wave functions are

$$\psi_\mathbf{k}(\mathbf{r}) = v^{-\frac{1}{2}} e^{i\mathbf{k}\cdot\mathbf{r}}, \quad \psi_{klm}(\mathbf{r}) = (\tfrac{1}{2}kR)^{-\frac{1}{2}} Y_l^m(\mathbf{r}) j_l(kr),$$

for $kR \gg l$, if we average the oscillating normalization integral of ψ_{klm} over k. It follows that

$$P(klm|\mathbf{k}') = 6\pi(k'R)^{-2}\delta(k-k')|Y_l^m(\mathbf{k}')|^2. \quad \text{(B.2)}$$

Apart from a normalization factor, $P(\mathbf{k}'|klm)$ is equal to $P(klm|\mathbf{k}')$. From the requirement that

$$\int (d\mathbf{k}')P(\mathbf{k}'|klm) = 1,$$

one obtains

$$P(\mathbf{k}'|klm) = k'^{-2}\delta(k-k')|Y_l^m(\mathbf{k}')|^2. \quad \text{(B.3)}$$

We now want to calculate the number of particles which exhibit relative momentum k and relative angular momentum l when colliding with particle No. 1:

$$N(kl|k_1l_1m_1) = \sum_{m=-l}^{l} N(klm|k_1l_1m_1) = \sum_m \int dk_2 \sum_{l_2m_2} P(klm|k_1l_1m_1k_2l_2m_2)N(k_2l_2m_2), \quad \text{(B.4)}$$

in to which we substitute (B.1). But

$$\int dk_2 \sum_{l_2m_2} P(\mathbf{k}_2'|k_2l_2m_2)N(k_2l_2m_2) = N(\mathbf{k}_2') = \begin{cases} v/(2\pi)^3 = R^3/6\pi^2, & \text{if } k_2' < k_F, \\ 0, & \text{if } k_2' > k_F, \end{cases} \quad \text{(B.5)}$$

if surface terms are neglected. Use of (B.2), (B.3), and (B.5) in (B.4) leads to

$$N(kl|k_1l_1m_1) = 2\pi^{-2}R(2l+1)\int_{|\mathbf{k}_1'-2\mathbf{k}'|<k_F} (d\mathbf{k}_1')(d\mathbf{k}_2')k_1^{-2}k^{-2} \times \delta(k-k')\delta(k_1-k_1')|Y_{l_1}^{m_1}(\mathbf{k}_1')|^2, \quad \text{(B.6)}$$

since

$$P(\mathbf{k}'|\mathbf{k}_1'\mathbf{k}_2') = \delta(\mathbf{k}' - \tfrac{1}{2}\mathbf{k}_1' + \tfrac{1}{2}\mathbf{k}_2').$$

The integral in (B.6) is evaluated by rotating the k' coordinate system so that its z axis coincides with k_1', over which we integrate later. The double integral is then seen to be zero for $k > \frac{1}{2}(k_1+k_F)$, and for $k < \frac{1}{2}(k_1+k_F)$,

$$\int d\Omega_{k_1'}|Y_{l_1}^{m_1}(\mathbf{k}_1')|^2 \int_0^{2\pi} d\varphi \int_{-\mu}^{1} d\cos\theta = 2\pi(1+\mu),$$

where

$$\mu = \text{lesser of } \left[1, \frac{k_F^2 - k_1^2 - 4k^2}{4kk_1}\right].$$

Consequently,

$$N(kl|k_1l_1m_1) = 4\pi^{-1}R(2l+1)(1+\mu), \quad \text{(B.7)}$$

which is independent of l_1 and m_1 and equal to $N(kl|\mathbf{k}_1)$.