Lower bounds on the ground-state energy and necessary conditions for the existence of bound states: The potential problem

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We consider a particle in a three-dimensional potential $V(\mathbf{r})$ or in a one-dimensional potential $V(x)$. We use a Green's-function approach to show that for many V's of interest one can obtain a necessary condition for the existence of a bound state below a specified energy that is somewhat stronger than the usual condition; furthermore, results can be obtained for $V(\mathbf{r})\neq V(r)$, under some special restrictions, which utilize an integral containing only one, not two, Green's functions.

I. INTRODUCTION

The power of the Rayleigh-Ritz principle and its generality—it provides an estimate of the ground-state energy that is of second order in the trial function and an upper bound, and is applicable to any system—are reflections of the fact that the Hamiltonian H is bounded from below. The determination of a lower bound on the ground-state energy, and the intimately connected problem of proving (where true) the nonexistence of a bound state, are very much more difficult; the results that have been obtained pertain almost exclusively to rather simple systems. We list a few such results, those relevant to the later discussion in this paper. This will at the same time establish a notation.

(i) For a particle of mass m in a central potential $V(r)$, a necessary condition for the existence of N_l bound states of angular momentum l is[1-3]

$$(2m/\hbar^2)\int_0^\infty r|V_-(r)|dr \geq (2l+1)N_l\ , \tag{1.1}$$

where

$$V_-(r)=\begin{cases} V(r) & \text{where } V(r)\leq 0 \\ 0 & \text{where } V(r)>0\ ; \end{cases} \tag{1.2}$$

it will be assumed throughout the paper that all potentials vanish at infinity. [For N_l large, the bound in Eq. (1.1) is rigorous but very poor; the strength of the potential will increase as N_l^2, not as N_l. The bound can give reasonable results for $N_l=1$.[4,5]]

(ii) The necessary condition for a central potential $V(r)$ to support N_l bound states of angular momentum l, where each state is bounded by at least an energy $E=-\kappa^2\hbar^2/(2m)$, is[2,3]

$$\int_0^\infty G_l(r,r;E)V_-(r)dr \geq N_l\ , \tag{1.3}$$

where the free-particle Green's function $G_l(r,r;E)$ is given by

$$G_l(r,r;E)=-(2m/\hbar^2)\kappa r^2 j_l(i\kappa r)h_l^{(1)}(i\kappa r)\quad (\leq 0)\ , \tag{1.4}$$

where j_l is a spherical Bessel function and $h_l^{(1)}$ is a spherical Hankel function of the first kind. [For $\kappa=0$, the inequality (1.3) reduces to (1.1).]

(iii) For a particle in a potential $V(\mathbf{r})$, where $V(\mathbf{r})$ need not be spherically symmetric, a lower bound on the ground-state energy which contains variational parameters can be obtained[3,6] from the Lippmann-Schwinger bound-state equation. (Since the reference is rather difficult to obtain, and since the proof is short, we give the proof here.) If there exist one or more bound states, and if the ground state has an energy $E=-\hbar^2\kappa^2/(2m)$, and a wave function $\psi(\mathbf{r})$, we have

$$\psi(\mathbf{r})=\int G(\mathbf{r},\mathbf{r}';E)V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}'\ , \tag{1.5}$$

where $G(\mathbf{r},\mathbf{r}';E)$, the free Green's function of energy E for a three-dimensional one-particle system, is given by

$$G(\mathbf{r},\mathbf{r}';E)=-\left(\frac{2m}{\hbar^2}\right)\frac{e^{-\kappa|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\quad (\leq 0)\ . \tag{1.6}$$

Since $\psi(\mathbf{r})$ is nodeless and can be taken to be positive, we can introduce a nodeless positive trial function $\psi_t(\mathbf{r})$ and rewrite Eq. (1.5) as[3,6]

$$\frac{1}{\psi_t(\mathbf{r})}\int G(\mathbf{r},\mathbf{r}';E)V(\mathbf{r}')\psi_t(\mathbf{r}')\frac{\psi(\mathbf{r}')}{\psi_t(\mathbf{r}')}d\mathbf{r}'=\frac{\psi(\mathbf{r})}{\psi_t(\mathbf{r})}\ . \tag{1.7}$$

With $\|\psi/\psi_t\|$ the maximum value of $\psi(\mathbf{r})/\psi_t(\mathbf{r})$, we then have, using the inequality $V(\mathbf{r})\geq V_-(\mathbf{r})$ and the fact that $G\leq 0$ and $GV_-\psi_t\geq 0$,

$$\left\|\frac{\psi(\mathbf{r})}{\psi_t(\mathbf{r})}\right\|=\max\left[\frac{1}{\psi_t(\mathbf{r})}\int G(\mathbf{r},\mathbf{r}';E)V_-(\mathbf{r}')\psi_t(\mathbf{r}')\frac{\psi(\mathbf{r}')}{\psi_t(\mathbf{r}')}d\mathbf{r}'\right]\leq\left\|\frac{\psi(\mathbf{r})}{\psi_t(\mathbf{r})}\right\|\max\left[\frac{1}{\psi_t(\mathbf{r})}\int G(\mathbf{r},\mathbf{r}';E)V_-(\mathbf{r}')\psi_t(\mathbf{r}')d\mathbf{r}'\right]\ ,$$

where max denotes the maximum over all values of $\mathbf{r}$. A lower bound is therefore provided by

$$\max[L(\mathbf{r};E)] \geq 1 , \tag{1.8}$$

where

$$L(\mathbf{r};E) \equiv \int G(\mathbf{r},\mathbf{r}';E)V_-(\mathbf{r}')\psi_t(\mathbf{r}')d\mathbf{r}'/\psi_t(\mathbf{r}) . \tag{1.9}$$

It is interesting to note that this lower bound is intimately connected with the standard result $E \geq \max(H\psi_t/\psi_t)$.

(iv) For the one-dimensional problem defined by $H=T+V(x)$, one obtains a bound on the ground-state energy E by first replacing $V(x)$ by $V_-(x)$, defined in analogy to the definition of $V_-(r)$ given in Eq. (1.2), and noting that $H>H_-=T+V_-(x)$. With $\psi_-(x)$ and E_- the normalized ground-state wave function and energy associated with H_-, and with x_1 defined as the (unknown) value of x for which $(|\psi_-(x)|)^2$ has its maximum, one then introduces

$$V_\delta(x) = \left[\int_{-\infty}^{\infty} V_-(x')dx'\right]\delta(x-x_1) \equiv -I\delta(x-x_1) , \tag{1.10}$$

and the normalized ground-state wave function $\psi_\delta(x)$ and energy $E_\delta=-(m/2\hbar^2)I^2$ associated with $H_\delta \equiv T+V_\delta(x)$. One then uses $\psi_-(x)$ as the trial function in a Rayleigh-Ritz determination of an upper bound on the ground-state of H_δ, and arrives at E_- as that upper bound.[4] Writing $H_-=H_\delta+(V_- - V_\delta)$, we thus have

$$E \geq E_- \geq E_\delta = -(m/2\hbar^2)I^2 . \tag{1.11}$$

(Note that it need *not* be the case that $H_- \geq H_\delta$. H_δ has one and only one bound state, with an energy E_δ, but H_- could have more than one bound state.)

We note that a knowledge of the number of bound states of a particle in a potential is not only of intrinsic interest, but plays a fundamental role in the determination of upper bounds on the scattering length.[7,8]

II. LOWER BOUNDS ON THE ENERGY

A. One-dimensional problems

1. A monotonicity theorem for a class of potentials

The lower bound E_δ on the energy for one particle in a one-dimensional potential $V(x)$, discussed in item (iv) of Sec. I, has recently been generalized[9] to the case of N bosons in one dimension with a pairwise interaction $V(x_i-x_j)$, it having been shown that $E(N) \geq E_\delta(N)$, where $E_\delta(N)$ is the (known) ground-state energy for the pairwise interaction $V_\delta=-I\sum_{i,j(i>j)}\delta(x_i-x_j)$, where, with $y \equiv x_i - x_j$, I is defined as

$$I = -\int_{-\infty}^{\infty} V_-(y)dy .$$

This interesting extension makes an attempt to improve the $N=1$ result more worthwhile.

It might be conjectured on physical grounds that, with E_λ the ground-state energy of a particle in a negative potential $V_\lambda(x)=\lambda V_-(\lambda x)$, and E, that for $V_-(x)$, one will have $E \geq E_\lambda$ for $\lambda>1$. (In the limit $\lambda \to \infty$, this reduces to $E \geq E_\delta$. Physically, one might conjecture that the more compact the potential, the more effectively the potential can act.) A somewhat analogous "compaction" theorem was given for the three-dimensional problem of an electron in the Coulomb field of two nuclei fixed at a separation r_{AB}. The ground-state energy $E(Z_A,Z_B;r_{AB})$ of the electron—the Coulomb potential energy between the two nuclei is *not* included—was shown to be a minimum for $r_{AB}=0$,[10] and, more generally,[11] to decrease monotonically as r_{AB} decreases.

A proof of the conjecture, if true, might be based on the approach used[11] in the proof that $dE(Z_A,Z_B,r_{AB})/dr_{AB}<0$, and then in the proof[9] that $E(N)>E_\delta(N)$. We will prove a less general result; thus we assume that there exists an x_0 such that

$$\frac{dV_-}{dx}\begin{cases}\geq 0 & \text{for } x>x_0\\ \leq 0 & \text{for } x<x_0 .\end{cases} \tag{2.1}$$

With $H(\lambda)=T+V_\lambda(x)=T+\lambda V_-(\lambda x)$, we have

$$\frac{\partial H(\lambda)}{\partial\lambda} = \frac{d}{dx}[xV_-(\lambda x)] . \tag{2.2}$$

With E_λ and $\psi_\lambda(x)$, the ground-state energy and wave function associated with $H(\lambda)$, the Hellmann-Feynman theorem then gives

$$\frac{dE_\lambda}{d\lambda} = \int \psi_\lambda^2(x)\frac{d}{dx}[xV_-(\lambda x)]dx = -\int xV_-(\lambda x)\frac{d}{dx}\psi_\lambda^2(x)dx , \tag{2.3}$$

where the range of integration is from $-\infty$ to ∞. It follows from the Schrödinger equation that

$$\frac{d^2}{dx^2}\psi_\lambda(x)\begin{cases}\geq 0 & \text{if } E \leq V_\lambda(x)\\ \leq 0 & \text{if } E \geq V_\lambda(x) .\end{cases}$$

Since $V(x)$ and therefore $V_\lambda(x)$ increase monotonically with $|x-x_0|$, there exists only one (continuous) region $\mathcal{R}$ in which $E \geq V_\lambda(x)$, and $d^2/dx^2\psi \leq 0$ in $\mathcal{R}$; it then follows, since the ground-state wave function ψ_λ is nodeless, that $\psi_\lambda^2(x)$ has only one maximum, and that the maximum lies within $\mathcal{R}$. Choosing the origin at the point at which $\psi_\lambda^2(x)$ has its maximum, we then have

$$\frac{d}{dx}\psi_\lambda^2(x)\begin{cases}\geq 0 & \text{if } x \leq 0\\ \leq 0 & \text{if } x \geq 0 .\end{cases}$$

We thus arrive at the monotonicity theorem,

$$\frac{dE_\lambda}{d\lambda} \leq 0 . \tag{2.4}$$

[We first obtained Eq. (2.4) by a graphic proof. The form of the proof as presented arose after a communication from Sokal.[12]]

As a minor but curious matter, we note that the result that $dE_\lambda/d\lambda \leq 0$ at $\lambda=1$ can be written as

$$\int \psi \left[\frac{d}{dx}(xV_-) \right] \psi\, dx = \int \psi \left[V_- + x\frac{dV_-}{dx} \right] \psi\, dx$$
$$= \int \psi (V_- + 2T)\psi\, dx \le 0 \ , \qquad (2.5)$$

using the virial theorem in the last step. Thus, for a bound state for a potential satisfying conditions (2.1) on $V_-(x)$, we have $-\langle V_- \rangle \ge 2\langle T \rangle$.

2. A lower bound on the energy by a Green's-function approach

The derivations of the (three-dimensional) result contained in Eq. (1.8) was based on a Green's-function technique. That approach can be immediately applied to a one-dimensional potential $V(x)$, provided suitable conditions are imposed on $V(x)$.

We consider a particle in a one-dimensional potential, which is symmetric, that is,

$$V(-x) = V(x) \ ,$$

and further, which satisfies

$$\frac{dV(x)}{d|x|} \ge 0 \ . \qquad (2.6)$$

The analog of Eq. (1.8) in the present one-dimensional case, for the choice $\psi_t(x) = 1$, gives

$$1 \le \max[L(x;E)] \ ,$$
$$L(x;E) \equiv \int G(x,x';E)V_-(x')dx' \quad (\ge 0) \ , \qquad (2.7)$$

where the one-particle free Green's function is given by

$$G(x,x';E) = -(2m/\hbar^2)e^{-\kappa|x-x'|}/(2\kappa) \quad (\le 0) \ .$$

To determine the maximum of $L(x;E)$, we consider

$$\frac{\hbar^2}{m}\frac{dL(x;E)}{dx} = \int_{-\infty}^{\infty} e^{-\kappa|x-x'|}V_-(x')\frac{x-x'}{|x-x'|}dx'$$
$$= \int_0^{\infty} e^{-\kappa u}[\,|V_-(u+x)| - |V_-(u-x)|\,]du \ . \qquad (2.8)$$

Since $|V_-(x)|$ decreases monotonically with $|x|$, and since $u \ge 0$, $|V_-(u+x)| - |V_-(u-x)|$ is nonpositive for $x \ge 0$ and non-negative for $x \le 0$. It follows that $L(x;E)$ has its maximum value at $x=0$, and the lower bound on the energy is given implicitly by

$$[2m/(\hbar^2\kappa)]\int_0^{\infty} e^{-\kappa x}|V_-(x)|dx \ge 1 \ . \qquad (2.9)$$

If we weaken the inequality (2.9) by using $\exp(-\kappa x) \le 1$, the result reduces to the explicit form

$$E \ge -(2m/\hbar^2)\left[\int_0^{\infty}|V_-(x)|dx\right]^2 = E_\delta \ , \qquad (2.10)$$

the result obtained previously[4] [without the restrictive conditions on $V(x)$ imposed by (2.6)] and discussed in item (iv) of Sec. I. The implicit bound provided by (2.9) is therefore better, when applicable, than the always applicable explicit bound provided by (2.10).

We will not go into any further details in connection with the present problem, but it is important for later purposes to note the following points. The use in (2.7) of

$$\max[\,|G(x,x';E)|\,] = |G(x',x';E)| = (m/\kappa\hbar^2)$$

leads immediately to $E \ge E_\delta$ [without imposing (2.6)], and this is presumably the best *explicit* result one can obtain for an arbitrary $V(x)$, but, as we have just seen, it is *not* necessarily the best (if implicit) result one can obtain if one imposes rather simple restrictions on $V(x)$, for one can then analytically maximize $L(x;E)$ rather than G. [One can, of course, maximize $L(x;E)$ analytically for a $V(x)$ which does not satisfy (2.6) if $L(x;E)$ can be evaluated analytically; one can, of course, always maximize $L(x;E)$ numerically.] For more complicated systems the possibility of maximizing $L(x;E)$ rather than G is not simply a matter of obtaining an improved lower bound, but can be essential if one is to obtain any lower bound at all. Thus, for a particle in three dimensions, $G_l(r,r';E)$ exists—see Eq. (1.4)—but the maximum value of $G(\mathbf{r},\mathbf{r}';E)$ of Eq. (1.6) is infinite; for a potential $V(\mathbf{r})$ which is not spherically symmetric one must consider $G(\mathbf{r},\mathbf{r}';E)$ and the maximization of $G(\mathbf{r},\mathbf{r}';E)$ alone is not possible. The maximum value of the relevant G for $V(\mathbf{r}) \ne V(r)$ for one particle in a space with dimension $D \ge 2$, or for two or more particle in a space with dimension $D \ge 1$, is also infinite.

B. Three-dimensional problems

For $V(\mathbf{r}) = V(r)$, one can readily obtain a bound on the energy[2,3] of a particle of angular momentum l. We proceed as in Sec. II A 2, but with $G(x,x';E)$ replaced by the free-particle Green's function of energy E and angular momentum l,

$$G_l(r,r';E) = -(2m/\hbar^2)\kappa r_< j_l(i\kappa r_<) r_> h_l^{(1)}(i\kappa r_>) \ , \qquad (2.11)$$

where $r_<$ and $r_>$ represent the smaller and larger of r and r'. Inspection of their power series shows that $i^{-l} r_< j_l(i\kappa r_<)$ is real and monotonically increasing and that $-i^l r_> h_l^{(1)}(i\kappa r_>)$ is real and monotonically decreasing. It follows that the maximum value of $G_l(r,r';E)$ as a function of r is at $r=r'$, and with E the ground-state energy for angular momentum l, we immediately obtain

$$\int G_l(r,r;E)V_-(r)dr \ge 1 \ , \qquad (2.12)$$

the special case ($N_l = 1$) of the result quoted in Eq. (1.3).

The bound in Eq. (2.12) makes no assumptions about $V(r)$. As for the one-dimensional case, it is natural to inquire if one can do better for particular assumptions about $V(r)$. We restrict our attention to the $l=0$ case, with

$$G_0(r,r';E) = -(2m/\hbar^2\kappa)\sinh(\kappa r_<)\exp(-\kappa r_>) \ . \qquad (2.13)$$

With $u_l(r) = r\psi_l(r)$, the integral equation $u_l = G_l V u_l$ for the radial wave function $u_l(r)$ can be written as

$$\psi_l(r;E)=\int G_l(r,r';E)V(r')\psi_l(r';E)r'dr'/r \ .$$

The necessary condition for the existence of a bound state of zero angular momentum and energy E then becomes

$$1\leq \max[L(r;E,l=0)] \ ,$$
$$L(r;E,l=0)\equiv \int_0^\infty G_0(r,r';E)V_-(r')r'dr'/r \ . \quad (2.14)$$

One finds

$$\frac{\kappa\hbar^2}{2m}r^2\frac{dL(r;E,l=0)}{dr} = -[(1+\kappa r)e^{-\kappa r}]\int_0^r r'\sinh(\kappa r')|V_-(r')|dr' + [\kappa r\cosh(\kappa r)-\sinh(\kappa r)]\int_r^\infty r'e^{-\kappa r'}|V_-(r')|dr' \ . \quad (2.15)$$

We now impose the condition

$$\frac{d|V_-(r)|}{dr}\leq 0 \quad \text{for all } r \ . \quad (2.16)$$

Since both square brackets in Eq. (2.15) are non-negative, we obtain an upper bound by replacing $|V_-(r')|$ by $|V_-(r)|$, its minimum value in the first integral and its maximum in the second. We can now perform the integrations; doing so, we arrive at

$$\frac{dL(r;E,l=0)}{dr}\leq 0 \ .$$

We thereby obtain the necessary condition, assuming the inequality (2.16),

$$(m/2\pi\hbar^2)\int_0^\infty (e^{-\kappa r}/r)|V_-(r)|4\pi r^2dr\geq 1 \ . \quad (2.17)$$

For $l=0$ and $N_l=1$, this is a stronger condition, when applicable, than the result quoted in inequality (1.3)—this follows from the fact that we made the best possible choice for r, namely $r=0$, and can be seen explicitly by noting that $1-\exp(-2x)\geq 2x\exp(-x)$—but the result in (1.3) presupposes no condition on $V(r)$.

If we start with $u_l=(G_lV_-)^2u_l$ rather than $u_l=G_lV_-u_l$ for a negative potential which satisfies (2.16), we arrive, for $l=0$, at

$$\max\left[\int\int G_0(r,r';E)V_-(r')G_0(r',r'';E)V_-(r'')r''dr'dr''/r\right]\geq 1 \ . \quad (2.18)$$

With L defined by (2.14), we rewrite this as

$$\max\left[\int G_0(r,r';E)\tilde{V}_-(r')r'dr'/r\right]\geq 1 \ , \quad (2.19)$$

where

$$\tilde{V}_-(r')\equiv V_-(r')L(r';E,l=0) \ .$$

Having assumed in Eq. (2.16) that $V_-(r)$ increases monotonically with r, we know that $L(r';E,l=0)$ decreases monotonically, and it follows that

$$\frac{d|\tilde{V}_-(r)|}{dr}\leq 0 \quad \text{for all } r \ . \quad (2.20)$$

Since (2.19) and (2.20) differ from (2.14) and (2.16) only in the replacement of $V_-(r)$ by $\tilde{V}_-(r)$, (2.17) remains valid if we replace $V_-(r)$ by $\tilde{V}_-(r)$. Making that replacement, and expressing $\tilde{V}_-(r)$ in terms of V_- and G_0, we arrive at

$$-(2m/\hbar^2)\int dr\int r'dr'e^{-\kappa r}V_-(r)G_0(r,r';E)V_-(r')\geq 1 \ . \quad (2.21)$$

Having chosen the best possible value of r, namely $r=0$, (2.21) is the best result obtainable starting from (2.18).

We can also obtain a lower bound on the ($l=0$) ground-state energy for a three-dimensional spherically symmetric potential from the bound for a one-dimensional potential. The reduced radial wave function for the $l=0$ state satisfies

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right]u(r)=Eu(r) \ ,$$

and the boundary condition $u(0)=u(\infty)=0$. The solution to this equation is equivalent to that with the one-dimensional potential

$$\tilde{V}(x)=\begin{cases}\infty & \text{if } x<0\\ V(x) & \text{if } x\geq 0 \ .\end{cases}$$

Since the one-dimensional ground-state energy is bounded by that in a δ function potential, we then have

$$E\geq -\frac{m}{2\hbar^2}\left[\int_0^\infty V_-(x)dx\right]^2 \ .$$

However, this lower bound is worse than that given in (1.3). [This is especially clear for the case $V(x)=V(-x)$. With D the dimensionality of the space, with E denoting ground-state energies and E^* denoting the first excited state, we have $E(D=3)=E^*(D=1)$, but our bound is not on $E^*(D=1)$; rather we are using $E(D=3)\geq E_\delta(D=1)$, where $E_\delta(D=1)$ is a bound on $E(D=1)$.] More generally, one can reduce the problem of the determination of bounds on D-dimensional problems to the problem of the determination of bounds on lower-dimensional problems, but the results so obtained are rather poor. A better bound on the ground-state energy for a spherically symmetric potential in a D-dimensional space can be obtained by applying the approach above with the (known) $l=0$ D-dimensional free Green's function.[13]

For a potential which satisfies

$$V_-(\mathbf{r})=V_-(-\mathbf{r}) \tag{2.22}$$

and

$$\frac{\partial V_-(\mathbf{r})}{\partial|x|}\geq 0,\quad \frac{\partial V_-(\mathbf{r})}{\partial|y|}\geq 0,\quad \frac{\partial V_-(\mathbf{r})}{\partial|z|}\geq 0\ ,$$

a simple lower bound on the ground-state energy can be obtained. Assuming that there exists a bound state with energy E, and proceeding in the same way as in obtaining (2.14), we have

$$\max[L(\mathbf{r};E)]\geq 1\ ,$$

where

$$L(\mathbf{r};E)=\int G(\mathbf{r},\mathbf{r}';E)V_-(\mathbf{r}')d^3r'\ .$$

The maximum value of $L(\mathbf{r};E)$ can be determined from a study of

$$\nabla L(\mathbf{r};E)=-\frac{2m}{\hbar^2}\int(1+\kappa q)\frac{e^{-\kappa q}}{4\pi q^2}\frac{\mathbf{q}}{q}V_-(\mathbf{q}+\mathbf{r})d^3q\ , \tag{2.23}$$

where $\mathbf{q}=\mathbf{r}'-\mathbf{r}$. Using the property that $V_-(\mathbf{q}+\mathbf{r})=V_-(-\mathbf{q}-\mathbf{r})$, the x component of Eq. (2.23) reduces to

$$\frac{\partial L(\mathbf{r};E)}{\partial x}=-\frac{m}{2\pi\hbar^2}\int_0^\infty dq_x\int_{-\infty}^\infty dq_y\int_{-\infty}^\infty dq_z(1+\kappa q)\frac{e^{-\kappa q}}{q^2}\times\frac{q_x}{q}[V_-(q_x+x,q_y+y,q_z+z)-V_-(q_x-x,q_y+y,q_z+z)]\ . \tag{2.24}$$

Since $\partial V(\mathbf{r})/\partial|x|\geq 0$, it follows that

$$\frac{\partial L(\mathbf{r};E)}{\partial|x|}\leq 0\ .$$

Similar results follow immediately for the partial derivatives with respect to $|y|$ and $|z|$; the lower bound on the ground-state energy is therefore determined by

$$\frac{m}{2\pi\hbar^2}\int\frac{e^{-\kappa r}}{r}[-V_-(\mathbf{r})]d^3r\geq 1\ . \tag{2.25}$$

We now compare the various lower bounds on the ground-state energy E. Taking the three-dimensional square-well potential

$$V(r)=\begin{cases}-V_0, & r\leq a\\ 0, & r>a\end{cases}$$

as a simple example—it satisfies condition (2.16)—we calculate the lower bound on E using the inequality defined by (1.8), and Eq. (1.9), with a one parameter trial function $re^{-\alpha r}$, and using inequalities (2.17), and (1.3) for $l=0$ and $N_l=1$. The lower bounds are compared with the exact E for two sets of arbitrarily chosen values of V_0a^2 in Table I. (We are interested only in qualitative results.) [It is to be expected that the trial function chosen above is a good approximation only for small values of $-(2m/\hbar^2)V_0a^2$.] Note that for each value of V_0a^2, the values decrease from left to right. Thus, as noted above, (2.17) is superior to (1.3), and, since $e^{-\alpha r}$ reduces to unity for $\alpha=0$, making the best choice of α guarantees that the result obtained from (1.8) is better than that from (2.17).

The truly interesting results are, of course, those associated with more than one particle. It must therefore be stressed that one-particle energy bounds can be of direct use in the analysis of many-body problems. Thus, for example, a bound[2] (upper in this case) on the sum of the negative energy eigenvalues for a particle in a potential $V(\mathbf{r})$ has been used[14] to obtain a lower bound on the kinetic energy of a many-body system, and the latter bound played a crucial role in the simplest proof which has been given[14] of the stability of matter. It should also be noted that the proof of the nonexistence of three-body systems can sometimes proceed via an intermediate (adiabatic approximation) stage in which two of the particles are held fixed; a prototype problem is an electron and two bare nuclei. The determination of a lower bound on the adiabatic energy in the intermediate stage is a one-body problem. The problem of the nonexistence of systems of two electrons and two bare nuclei can also be reduced to the study of a one-body problem. This adiabatic approach has been studied in some detail.[15] Finally, we note that the necessary condition and lower bound provided by (1.8), and Eq. (1.9), while perhaps not there the best approach, is applicable to many-body systems.

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TABLE I. Comparison, for two square-well potentials, of various lower bounds on the ground-state energy with the exact numerical value and with one another. The energies are in rydbergs.

$-(2m/\hbar^2)V_0a^2$	Exact	Eq. (1.8)	Eq. (2.17)	Eq. (1.3)
2.25	−0.075	−0.085	−0.19	−0.27
25	−0.21	−0.46	−0.50	−6.0

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