

On the non-existence of bound states

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The Rayleigh-Ritz theorem — I believe that Ritz had little to do with the development of the theorem, though in the interest of full disclosure let me note that Rayleigh is one of my heroes — provides an upper bound \bar{E}_{gd} on the ground-state energy E_{gd} for a remarkably wide range of systems. It assumes only that there exists a potential V . V can be angle-dependent, spin-dependent, or non-local, for example, and the system can comprise an arbitrary number of particles. What the theorem can *not* do is prove (when true) that there is no bound state. Let E_{ref} be the appropriate reference energy level. (In an attempt to prove, for example, that an e^+ cannot be bound to a hydrogen atom, the reference level would be the ground-state energy of the H atom.) If one cannot find a trial function Ψ_t for which \bar{E}_{gd} , computed using Ψ_t , lies below E_{ref} , it does not prove that there is no bound state; a better Ψ_t might prove that there is a bound state. There is no margin of error; a proof that $\bar{E}_{gd} - E_{ref} < \epsilon$, where ϵ is an arbitrarily small positive number, tells us nothing about whether or not a bound state exists. What is needed is not an upper bound on $E_{gd} - E_{ref}$ but a lower bound. After a discussion of one-body problems, we will turn to the many-body problem; it has been shown that the adiabatic approximation provides a lower bound on $E_{gd} - E_{ref}$ and can be used to prove that certain bound states cannot exist.

Apart from the problem of a particle of mass m in a potential $V(r)$, there is little in the literature on the proof of the non-existence of a bound state. For the potential problem one does have the result that with $V_-(r) \equiv V(r)$ for $V(r) \leq 0$ and $V_-(r) = 0$ for $V(r) > 0$,

$$(2m/\hbar^2) \int_0^\infty |V_-(r)| r dr > 2l + 1$$

is a necessary condition for the existence of a bound state of angular momentum $l\hbar$. Alternatively, one can numerically determine the zero energy wave function $\Psi_0(r)$ defined by the one-body Schroedinger equation and standard boundary conditions; if $\Psi_0(r)$ does not pass through zero (at other than $r = 0$ and $r = \infty$), there is no bound state.

There is a simple result for a particle in a one dimensional potential $V(x)$. If $\int_{-\infty}^\infty V(x) dx < 0$, a bound state exists [29; p199].

There is a related result, but one which is not concerned with the question of the existence of a bound state. Let $V_-(x)$ be defined in a manner analogous to the definition of $V_-(r)$, and $\Psi_-(x)$ be the ground state wave function for $T + V_-(x)$. We now compactify $V_-(x)$, introducing

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

where x_1 is the (unknown) value of x for which $|\Psi_-(x)|^2$ has its maximum. Then one can readily show that

$$E > E_\delta = -(m/2\hbar^2)I^2.$$

Of all potentials $V(x)$ with a fixed value of I , the δ function version gives the lowest energy. Roughly speaking, one can then efficiently pile up the wave function at the location of the δ function [29; p200].

We turn now to many-particle systems [29, 41, 51, 55,56]. Consider, for example, the question of whether or not a positron e^+ can be bound to a hydrogen atom. Our approach is to reduce the problem to a sequence of two one-body problems. Thus, we start by using the adiabatic approximation. We freeze the e^+ at a particular point \mathbf{r}_+ , with the (fixed) proton p defining the origin, and determine the energy $\mathcal{E}(r_+)$ of the e^- in the potential generated by the p and the e^+ . We then determine the energy \underline{E} of the e^+ in the potential $e^2/r_+ + \mathcal{E}(r_+)$. \underline{E} is a *lower* bound on the ground-state energy of the hydrogen- e^+ system, as we will discuss in a moment. If, then, \underline{E} lies above the ground-state energy of the hydrogen atom, there is no e^+ -hydrogen atom bound state.

One can see why \underline{E} is a lower bound by comparing the adiabatic approximation with the Rayleigh-Ritz approach. In the latter case one chooses a trial function Ψ_t which contains parameters which are varied to obtain the best upper bound \bar{E}_{gd} on the ground-state energy E_{gd} . The introduction of additional parameters in Ψ_t allows greater freedom in Ψ_t , and gives a better (that is, lower) upper bound. But in freezing the e^+ at a particular point, we have allowed the e^- an arbitrary amount of time to adjust to the location of the e^+ , that is, we have given the e^- *more* freedom than is truly allowed, and we therefore obtain a lower bound on E_{gd} .

In fact, the above procedure, which can be useful in other situations, is not capable of proving the non-existence of a bound state of e^+ and a hydrogen atom. (The lower bound on E_{gd} that one obtains is not good enough.) A “proof” does follow if one does not freeze the e^+ at a particular point \mathbf{r}_+ in space but at a fixed distance r_+ from the p , that is, on the surface of a sphere of radius r_+ . A significant feature is that a margin of error is allowed. One cannot obtain the exact ground-state energy of the e^+ -hydrogen atom for the e^+ fixed on the sphere. However, if one gives the e^+ a mass twice its true value, and if no bound state is found for the increased mass, then surely the very slight error in the (variational) estimate of the ground state of the system can be ignored. (This is a physicist talking, not a mathematician.) For the e^+ frozen on the surface of a sphere, the e^- can better adjust to the position of the e^+ than it can for the real problem, but it can less easily adjust than it can for the e^+ frozen at a fixed point. Freezing the e^+ at fixed r_+ rather than fixed \mathbf{r}_+ therefore provides an improved lower bound [62].

(The analysis of $e^+ + \text{H}$ with the e^+ frozen on the surface of a sphere entailed a fair effort. The effort was undertaken because at that time the existence or non-existence of a bound state played a role in the dispersion theoretic analysis of the scattering of e^+ by H.)

As a second example of too much freedom, consider a helium atom in its ground state, and let the e^- coordinates in the zero orbital angular momentum ground state be r_1 , r_2 , and r_{12} . r_{12} is not totally independent of r_1 and r_2 . If we take r_{12} to be a totally independent variable, the exact solution will be below the true ground-state energy.

In the analysis above we effectively obtained the other (lower) bound on the ground state energy. The same technique can sometimes be used to obtain the other (upper) bound on the scattering length[76].

We now consider the possibility of a bound state of e^+ and a helium atom. The ground-state energy of two electrons for the alpha particle and e^+ at fixed points a distance r_+ apart is known, and it is easily shown that the resultant one-body problem does not allow a bound state.

The results in [154] and [155] are somewhat technical and contain many theorems, and one has to read the paper — a summary would be a mapping on a scale of roughly one to one. The essential idea is to find scaling laws that enable one to use known energies for one or two electrons in two fixed centers with fixed charges to obtain energies for different fixed charges. We can then use the adiabatic approximation to reduce the problem to a one-body potential problem, and to possibly prove that no bound state can exist. Some systems which have been shown to be incapable of forming composite bound states are listed in Table I of [155].

There is some overlap between this contribution and those of Yukap Hahn and Mike Lieber.