New lower bounds for quantum Hamiltonians

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A new variational principle is presented which provides a lower bound to the eigenvalues of a general quantum Hamiltonian. Applications are made to ground and excited states in Schrödinger theory. The variational principle leads naturally to localized (classical-like) states that nevertheless contain effects due to quantum fluctuations in a variational manner. Except for possible exceptional end-point solutions, these "classical" or "semiquantum" configurations provide lower bonds to the true eigenvalue.

I. INTRODUCTION

In this paper a new approach of the problem of taking a classical-type limit of quantum theories will be presented. In contrast to the conventional approach, the method used here does not neglect the effects of quantum fluctuations on the energy but approximates them in a variational way. The resulting wave functions are localized but the method is not a direct expansion in $\hbar$. The resulting energy eigenvalues for ground and excited states are usually lower bounds to their corresponding quantum values.

Bargmann[1] has discussed an interesting set of bounds for the expectation value of the kinetic energy. For normalizable wave functions, he has discussed in detail inequalities of the form

$$\int d^n x \,|\nabla\phi|^2 \geq \tfrac{1}{4}(n+m)^2\langle\phi|r^m|\phi\rangle^2/\langle\phi|r^{2m+2}|\phi\rangle\,, \tag{1.1}$$

where n is the number of space dimensions and m is an arbitrary parameter. He applied this to the problem of binding in a Coulomb potential and derived a simple lower limit to the ground-state energy which is exact for the choice $m=-1$. In general, for a given potential, the allowed range of m that produces a nontrivial bound is quite restricted. For example, if m is too negative, then the integrals will diverge at the origin, etc.

This type of inequality is a generalization of the familiar uncertainty-principle arguments used to estimate the kinetic energy term. The use of such inequalities forms the basis for the method presented here.[2] We shall discuss first its application of Schrödinger-type problems and then briefly explore the physical interpretation of the solutions.

In Sec. II, a generalized inequality on the kinetic energy is derived following the work of Bargmann and the general variational problem for a lower bound on the total energy eigenvalue is derived.

In Sec. III the best lower bounds are shown to come from wave functions which are localized at one point and yet which have effects of quantum fluctuations in the energy estimate. Lower bounds for the first few states of λx^2, λx^4, and $\lambda(x^2-f^2)^2$ potentials are worked out as examples. A perturbation method is developed in the Appendix which systematically improves these results. Section IV discusses an alternative method for obtaining lower bounds that does not always lead to localized wave functions.

Some conclusing remarks are then given, and an interpretation of the "classical" value of the equilibrium coordinate is discussed in terms of quantum-mechanical expectation values. The applications of these methods to field theories on a lattice will be made in a subsequent paper.[3]

II. GENERALIZED INEQUALITY

We want to find a lower bound on the energy of the one-dimensional Hamiltonian

$$H = -\frac{d^2}{dz^2} + V(z)\,.$$

The energy may always be expressed in terms of the exact, normalized wave function Ψ by

$$E = \left(\frac{d\Psi}{dz}, \frac{d\Psi}{dz}\right) + (\Psi, V\Psi)\,.$$

As suggested by Bargmann,[1] the kinetic energy may now be approximated by using the Schwarz inequality

$$\left(\frac{d\Psi}{dz}, \frac{d\Psi}{dz}\right)(g\Psi, g\Psi) \geq \left[\mathrm{Re}\left(g\Psi, \frac{d\Psi}{dz}\right)\right]^2, \tag{2.1}$$

which holds for any function $g(z)$. Because every eigenvalue has at least one real eigenfunction, we may assume Ψ is real. It is then convenient to choose g real so that

$$\mathrm{Re}\left(g\Psi, \frac{d\Psi}{dz}\right) = -\frac{1}{2}\left(\Psi, \frac{dg}{dz}\Psi\right).$$

Now let ψ be an arbitrary normalized function and

define the functional

$$E_L(\psi) \equiv \frac{(\psi, g'\psi)^2}{4(\psi, g^2\psi)} + (\psi, V\psi). \tag{2.2}$$

When the exact eigenfunction Ψ is known, one has

$$E \geq E_L(\Psi).$$

Note that for an arbitrary ψ, $E_L(\psi)$ can be smaller or larger than E. If, however, one varies (2.1) over all functions ψ, a lower bound on E is obtained because

$$E \geq E_L(\Psi) \geq \min E_L(\psi). \tag{2.3}$$

Note that, varying over all functions, ψ will only give a lower bound for the ground-state energy. By restricting the class of admissible wave functions, for example by fixing the number of nodes of ψ, one obtains a lower bound to the eigenvalue of H whose eigenfunction lies within that class. These statements are true regardless of the choice made for g. Obviously the quality of the lower bound does depend on the choice of g. In making this choice it is helpful to note that if

$$g(z) \propto \frac{\Psi'(z)}{\Psi(z)}, \tag{2.4}$$

then the inequality (2.1) used to bound the kinetic energy becomes an equality. Thus a good guess for Ψ leads immediately to a choice for g. Note also that since acceptable wave functions will usually have definite parity, the g must have negative parity.

There are two different ways to actually minimize $E_L(\psi)$. One may functionally differentiate with respect to ψ; this leads to the localized minima discussed in Sec. III. Alternatively, one may minimize (2.2) with respect to the matrix elements $(\psi, g'\psi)$, etc. This approach is discussed in Sec. IV.

III. LOCALIZED MINIMA

To find a lower bound on E it is necessary to find the exact minimum of $E_L(\psi)$. (This is in contrast to the familiar Rayleigh-Ritz upper-bound calculations where just varying a few parameters in a trial function gives a bound.) Fortunately, it is quite easy here to find the minimum of $E_L(\psi)$ provided $g(z)$ has been wisely chosen. (See Sec. III C below for choices of g.) Minimizing over normalizable ψ gives

$$\left[\frac{\langle g'\rangle}{2\langle g^2\rangle} g(z) - \frac{\langle g'\rangle^2}{4\langle g^2\rangle^2} g^2(z) + V(z)\right]\psi(z) = E_L\psi(z). \tag{3.1}$$

This equation can only be satisfied at discrete values of z. Thus

$$|\psi(z)|^2 = \delta(z - x), \tag{3.2}$$

where the parameter x characterizes ψ. The eigenvalues are then

$$E_L(x) = \frac{1}{4}\left(\frac{g'(x)}{g(x)}\right)^2 + V(x) \tag{3.3}$$

for any value of x. The lowest eigenvalue is found by minimizing (3.3) with respect to x. The localized states described by (3.2) are classical-like (localized) but they include an estimate of the kinetic energy (or quantum fluctuations in position). This result may be considered a more powerful version of the familiar uncertainty-principle estimates of ground-state energies. It provides a lower bound to that energy provided g has been wisely chosen. This can be tested by varying g (or parameters in g) in any particular application.

A. Ground-state examples

Let us now investigate the ground state of two simple potentials: $V = \lambda x^2$ and $V = \lambda x^4$. In both cases the ground-state wave function is expected to have a maximum at $x = 0$ and no nodes. Consequently $g_0(x) = x$ is suggested by (2.4). The resulting minimization problem is

$$E_L(x) = \frac{1}{4x^2} + V(x).$$

For a harmonic force, $V = \lambda x^2$, one finds $E_L(\min) = \sqrt{\lambda}$, which is actually the exact energy. For the anharmonic force, $V = \lambda x^4$, one finds $E_L(\min) = \frac{3}{4}\lambda^{1/3}$, whereas the exact answer is about $1.06\lambda^{1/3}$. Although the percentage error here is large, it should perhaps be compared to the usual classical minimum, i.e., zero.

In order to improve the lower bound for the anharmonic force, one might choose $g_0(x) = x^2$. The minimization problem is then

$$E_L(x) = \frac{1}{x^2} + V(x).$$

For $V = \lambda x^4$ one finds $E_L(\min) = \frac{3}{2}(2\lambda)^{1/3}$. This is certainly not a lower bound to the ground-state energy of $1.08\lambda^{1/3}$. The error here is not hard to find. The original functional to be minimized was (2.2), i.e.,

$$E_L(\psi) = \frac{(\psi, z\psi)^2}{(\psi, z^4\psi)} + \lambda(\psi, z^4\psi).$$

The minimum of this quantity is actually achieved by a ψ which has definite parity so that the kinetic energy vanishes, and which then minimizes the potential energy separately. For such a ψ, $E_L(\psi)$ can be made arbitrarily near to zero. Thus $g_0(x) = x^2$ is not an acceptable choice because its minima

are of a trivial end-point type and the energy is no improvement over the purely classical value. We now investigate how to avoid such minima.

B. The choice of g

The problem of minimizing $E_L(\Psi)$ over all normalized functions Ψ is intimately connected with the choice made for $g(x)$. If a poor choice is made for g then there are functions Ψ which make the kinetic energy term in (2.4) arbitrarily small. The resulting minimum is then just the classical minimum and is trivial. Such end-point solutions to the variational problem are of several types, the simplest two are

$$\text{I: } (\psi, g^2\psi) \to \infty, \qquad \text{II: } (\psi, g\psi) \to 0. \tag{3.4}$$

Type I always results from the behavior of $g(x)$ at $x \to \pm\infty$. [A divergence of $g(x)$ at any finite point would only restrict Ψ to vanish at that point and would not lead to a divergence of $\langle g^2 \rangle$.] If $g^2(x)/V(x)$ is bounded as $x \to \pm\infty$ then the trivial extrema of type I are easily avoided. Type II can be avoided by choosing a $g(x)$ with the property

$$g'(x) > c,$$

where c is some positive constant. Note that the constraint must hold for all x. If, for instance, $g'(x) = 0$ at one value of x, then a fixed Ψ which is concentrated at that value will minimize $E_L(\Psi)$ in a trivial (i.e., classical) fashion.

Choosing a function g that avoids such end-point minima only guarantees that the lower bound on the kinetic energy will not be trivial, e.g., zero. From all such functions g we would like to choose one which actually gives the greatest lower bound. If we actually knew the exact eigenfunction Ψ, then the best choice for g would be (2.4), for it makes the inequality (2.1) into an equality and it converts the variational equation (3.1) into the original Schrödinger equation. Obviously Ψ is unknown, but a reasonable guess for Ψ may lead to a g given by (2.4) that produces a useful lower bound.

An alternative method is to build some knowledge of Ψ into g by choosing the poles and zeros of g judiciously. This is particularly simple for a potential that is a polynomial in x^2 with positive coefficients. The wave function for the nth excited state in such a potential has n nodes $(d_2, d_4, \ldots, d_{2n})$ and $n+1$ extrema $(d_1, d_3, \ldots, d_{2n+1})$ which alternate as follows:

$$d_1 < d_2 < \cdots < d_{2n} < d_{2n+1}. \tag{3.5}$$

This suggests choosing

$$g_n(x) \frac{(x-d_1)(x-d_3)\cdots(x-d_{2n+1})}{(x-d_2)(x-d_4)\cdots(x-d_{2n})}. \tag{3.6}$$

Note that because of the symmetry of the potential about $x = 0$,

$$d_n = 0, \quad d_{n+1-j} = -d_{n+1+j}.$$

It is easy to check that this g does not lead to either of the trivial end-point solutions (3.4). Type I is avoided because g^2/V is bounded as $x \to \pm\infty$. To see that type II does not occur, observe that (3.6) may be written

$$g\hat{n}(x) = x - c - \frac{D_1}{x-d_2} - \frac{D_2}{x-d_4} - \cdots - \frac{D_n}{x-d_{2n}}.$$

Furthermore, all the constants D_j are positive because of the alternation (3.5) of nodes and extrema. Consequently $g'(x) > 1$ for all x and can never vanish.

C. Further examples

Let us now derive lower bounds for the excited states of the λx^2 and λx^4 potentials. For the first excited state both wave functions are expected to have a node at $x = 0$ and extrema at $x = \pm a$. Consequently we take

$$g_1(x) = \frac{x^2 - a^2}{x},$$

so that

$$E_L(x) = \frac{1}{4x^2}\left(\frac{x^2+a^2}{x^2-a^2}\right)^2 + V(x). \tag{3.7}$$

It is necessary to minimize this quantity with respect to x and maximize with respect to a. For monotonically increasing potentials, there are generally two minima in x: one for $x^2 < a^2$ and one for $x^2 > a^2$. For large a the former approaches the ground-state bound and for small a the latter approaches this value. Hence there is an optimum value of a and it is achieved when the values of $E_L(\min)$ for $x^2 < a^2$ and for $x^2 > a^2$ are equal. For $V = \lambda x^2$ this procedure can be carried out analytically and one finds $a^2 = 1/\sqrt{\lambda}$ and $E_L(\min) = 3\sqrt{\lambda}$, which is the exact answer. For $V = \lambda x^4$ the bound must be found numerically. The result is $a^2 = 0.75/\lambda^{1/3}$ and $E_L(\min) = 3.73\lambda^{1/3}$. The exact value for this level is less than $3.80\lambda^{1/3}$.

The wave functions for the second excited states are expected to have nodes at $x = \pm b$ and extrema at $x = 0$, $\pm c$, and $c > b$. Consequently we take

$$g_2(x) = \frac{x(x^2 - c^2)}{(x^2 - b^2)}.$$

Then

$$E_L(x) = \frac{1}{4x^2}\left(1 + \frac{2x^2}{x^2-b^2} - \frac{2x^2}{x^3-c^2}\right)^2 + V(x). \tag{3.8}$$

For $V = \lambda x^2$ the optimum values are $b^2 = 1/2\sqrt{\lambda}$, $c^2 = 5/2\sqrt{\lambda}$, and $E_L(\min) = 5\sqrt{\lambda}$, as expected. For

$V=\lambda x^4$, one finds $b^2\approx 0.33/\lambda^{1/3}$, $c^2\sim 1.50/\lambda^{1/3}$, and $E_L(\min)=7.30\lambda^{1/3}$. The exact energy of this level is less than $7.46\lambda^{1/3}$.

Let us now try to improve the above estimates. The method to be described below will work for any excited state in a general potential, but we shall discuss explicitly only the ground state in the λx^4 case. The original quantum Hamiltonian can be written as one-half the sum of two independent oscillators:

$$2H=-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+\lambda x^4+\lambda y^4 .$$

In the x-y plane, the potential rises most rapidly along the 45° lines. This suggests changing variables to $u=(x+y)/\sqrt{2}$ and $v=(x-y)/\sqrt{2}$. The kinetic energy can now be bounded in the usual way in terms of these new variables and the effective Hamiltonian is

$$2H_L(y)=\frac{1}{4u^2}+\frac{1}{4v^2}+\tfrac{1}{2}(u^4+v^4+6u^2v^2) .$$

The minimization is easily accomplished with the result

$$H_L(\min)=\tfrac{3}{4}(2\lambda)^{1/3}\cong 0.945\lambda^{1/3} , \tag{3.9}$$

which is a substantial improvement over our previous result in Sec. II A.

Using the above procedure for a lower bound to E and a standard variational upper-bound estimate with Gaussian trial functions of width $\langle x^2\rangle=y^2$, an amusing result can be derived for the ground-state energy, if V is symmetric:

$$\min_y\left[\frac{1}{4y^2}+\frac{1}{2}W(2y^2)\right]\le E \le \min_y\left[\frac{1}{4y^2}+\frac{1}{y}W\left(y^3\frac{\partial}{\partial y}\right)y\right] ,$$

where $V(x)=W(x^2)$.

D. Potentials with two minima

We will now discuss the potential

$$V(x)=\lambda(x^2-f^2)^2 ,$$

which will prove to be of some interest in the field theory case. If f^2 is large, then the wave function in such a potential will be peaked at $x^2\sim f^2$ and will be small near the origin. For this situation consider the simple trial function

$$\psi_0=x^{2n}e^{-x^2/2a} ,$$

which leads to

$$g=x-2na/x .$$

and

$$E_L(x)=\frac{1}{4}\left(\frac{1}{x}+\frac{2x}{2na-x^2}\right)^2+\lambda(x^2-f^2)^2 . \tag{3.10}$$

Because ψ_0 vanishes at the origin, one is not guaranteed that this always provides a lower bound for the ground-state energy but it should be a good approximation.

The optimum value of $(2na)$ is clearly near f^2 (actually slightly larger) in order to move the minimum away from $x^2=f^2$ where the potential vanishes. Consider the simplest choice $2na=f^2$ so that

$$E_L(x)=\frac{1}{4x^2}\left(\frac{x^2+f^2}{x^2-f^2}\right)^2+\lambda(x^2-f^2)^2 . \tag{3.11}$$

Note that this Hamiltonian satisfies a scaling relation also satisfied by the exact quantum Hamiltonian,

$$E_L(x;\lambda,f^2)=\lambda^{1/3}E_L[x;1,\lambda^{1/3}f^2] , \tag{3.12}$$

a result guaranteed by choosing $(2na)$ proportional to $f^2J(\lambda f^6)$ where $J(\lambda f^6)$ is an arbitrary function with $J(\infty)=1$.

If one chooses $J=1$, $E_L(\min)$ turns out to be a lower bound to the true ground-state energy. However, if one minimizes with respect to x in (3.11) and then maximizes with respect to $J(\lambda f^6)$, the resultant value of E_L is a lower bound to the first excited state. One already knows from our earlier discussion that this optimum $J(z)$ has the limiting behavior $J(\infty)=1$ and $J(z)\sim 0.75/z^{1/3}$ for $z\sim 0$ (see Sec. III C).

The absolute minimization of Eq. (3.11) evidently should be done numerically. An excellent analytic approximation to the solution exists which is never in error by more than 1% for any value of f^2:

$$E_L(\min)\cong(\lambda)[4(\lambda)^{3/2}f^2+\tfrac{9}{16}]^{1/2} .$$

The comparison with the exact solution to the quantum-mechanical problem can easily be made. As was discussed before, $H_L(\min)$ falls below the exact value by ~30% at $f^2=0$ and by ~10% at $f^2=1.0$. For larger values of f^2 this error rapidly approaches zero. This result seems to be a lower bound to the true ground-state energy but this a fortuitous result. It is guaranteed for $f^2=0$ and $f^2=\infty$ but not for intermediate values. What we wish to emphasize here is that the choice of a g that arises from a reasonable wave function gives a good approximation to the energy level.

IV. RIGOROUS LOWER BOUNDS

We will now discuss a completely different method of minimizing the functional E_L in (2.2). Instead of minimizing with respect to the functions ψ we will now minimize with respect to the matrix elements. Consider again the potentials λx^2 and λx^4 (or more generally any polynomial in x^2

with positive coefficients). Because the ground-state result is the same as before, we turn immediately to the first excited state and choose

$$g_1(x) = \frac{x^2 - a}{x} . \tag{4.1}$$

Consequently,

$$E_L = \frac{\langle 1 + a/x^2 \rangle^2}{4\langle x^2 - 2a + a^2/x^2 \rangle} + \langle V \rangle . \tag{4.2}$$

Now define two variables $y = \langle 1/x^2 \rangle$ and $z = \langle x^2 \rangle$. Of course these variables are not completely independent; they must satisfy $yz \geq 1$. The minimization with respect to parameters that are restricted to satisfy such inequalities is easily carried out by using the method of Lagrange inequality multipliers.[4] Introducing the positive semidefinite multiplier ν, the lower bound Hamiltonian for the first excited state becomes

$$E'_L \geq \tfrac{1}{4}(1 + ay)^2 (z - 2a + a^2 y)^{-1} + V(z) - \nu(zy - 1) , \tag{4.3}$$

where the Schwarz inequality has been used to bound the potential. By setting $dE'_L/dy = 0$ one can search for minima in the interior of the allowed region ($yz > 1$ and $\nu \equiv 0$) or on the boundary ($yz = 1, \nu > 0$). For the interior region one finds

$$y = (5a - 2z)/a^2 ,$$

and the interior constraint $5 - \sqrt{17} \leq 4z/a \leq 5 + \sqrt{17}$ insures that $yz \geq 1$. If this is true, then

$$E'_L \geq \frac{3}{a} - \frac{z}{a^2} + V(z) .$$

One must now minimize with respect to z and if the interior constraint is satisfied then maximize with respect to a.

For the (almost) harmonic potential $V = z^{1+\epsilon}$, one finds, as $\epsilon \to 0$, $a \to 1$ and $E_L \geq 3$, the exact answer. For the anharmonic potential one finds a minimum at $z = 1/2a^2$ and a maximum is $1/a^3 = 3$. Therefore $z/a = \frac{3}{2}$ which is on the interior, and the energy is

$$E_L(\min) = \tfrac{9}{4}(3\lambda)^{1/3} \cong 3.245\lambda^{1/3} , \tag{4.4}$$

which is ~15% below the exact value.

One may wonder from the above example how $zy > 1$ in the kinetic term but that $\langle x^4 \rangle = \langle x^2 \rangle^2$ in the potential term, since the latter condition seems to imply a localized wave function. The wave function evidently has the limiting form

$$|\psi(x)|^2 \simeq Ax^2\delta(x) + B\delta(x^2 - 1/2a^2) .$$

The first term only contributes to the expectation value of $\langle 1/x^2 \rangle = y$ and not to any other.

A similar exercise can be carried out for the second (and even higher if you wish) excited states. For the second state the energy bound is (if the minima lies in the interior region)

$$E_L \geq \frac{5}{a} - \frac{z}{a^2} + V(z) .$$

This again gives the exact result for the harmonic case, and for the anharmonic case yields an energy which is ~15% below the exact answer. We have obtained similar results for other simple polynomial potentials. If there are negative coefficients in the potential, say of the x^{2N} term, then this can be handled by choosing $g(x)$ so that a $\langle x^{2N} \rangle$ term occurs explicitly in the kinetic energy estimate.

V. CONCLUSION

The interpretation of the solutions, x, to the semiquantum theory are clearly not to be identified as an approximation to $\langle x \rangle$ in the exact quantum treatment (although perhaps a more reasonable choice would be $\langle x^2 \rangle^{1/2}$). To explore this in more detail let us study a one-dimensional problem with $V(x) = V(-x)$, and write

$$H = \tfrac{1}{2}\pi^2 + V(x) + Jx , \tag{5.1}$$

hence

$$\langle x \rangle = \left. \frac{dE(J)}{dJ} \right|_{J=0} \tag{5.2}$$

by the Feynman-Hellman theorem.

In the semiquantum approximation, the natural choice for $J = 0$ is an even $V(x)$ and even $\pi^2(x)$. Thus

$$H_L = \tfrac{1}{2}\pi^2(x) + V(x) . \tag{5.3}$$

Assume that there are two solutions to this minimization problem at $x = \pm x_0$, say.

If the term Jx is now added to H_L (with J small), it is clear that the optimum $\pi^2(x)$ must also be modified to include the effect of this symmetry-breaking term. In fact, it is clear that the change in $\pi^2(x)$ must be such that the root near $+x_0$ is still equal to the one near $-x_0$ (otherwise one would be lower and hence not optimum). Hence let us write, to first order in J,

$$H_L = \tfrac{1}{2}\pi^2(x + Jb) + V(x) + Jx . \tag{5.4}$$

The problem is to find the value of x that minimizes H_L and then find the (optimum) value of b, i.e., the one that maximizes H_L. First, minimize with respect to x:

$$0 = \frac{\partial H_L}{\partial x} = \tfrac{1}{2}\frac{d\pi^2}{dx}(x + Jb) + \frac{\partial V(x)}{\partial x} + J .$$

Expanding this solution to first order in J around x_0, we find

$$x = x_0 + Jx_1 + \cdots$$

which yields the first-order solutions

$$x_1 = -\left(1 + b\frac{d^2\pi^2(x_0)}{dx_0^2}\right)\Big/\frac{d^2H(x_0)}{dx_0^2}$$

$$= -(1 + b\pi_0^{2\prime\prime})/H_0^{\prime\prime},$$

and the energy becomes

$$E_L = H_L(x_0)\big|_{J=0} + J(x_0 - bV_0') + O(J^2). \tag{5.5}$$

Requiring that E_L be the same at $\pm x_0$ then fixes the optimum b to be $b = x_0/V_0'$, which is an even function of x_0, as it should be. Thus for this optimum b,

$$E_L = H(x_0)\big|_{J=0} + O(J^2)$$

and

$$\langle x\rangle = 0, \tag{5.6}$$

as expected. And also, as might be anticipated, if one adds a term Jx^2 to H_L, and carries through a similar argument, the result is $\langle x^2\rangle = x_0^2$.

In a later treatment of lattice field theory, we will find a nonzero classical-like solution to the field equation $\phi_c(x)$. These are therefore not to be interpreted as $\langle\phi(x)\rangle = \phi_c$, which would imply symmetry breaking, but rather as $\langle\phi(x)^2\rangle = \phi_c^2$.

In this paper we have presented a new and simple approach to the problem of finding lower bounds to the eigenvalues of quantum Hamiltonians. This approach leads very naturally to classical-like states that are localizable. The bounds are variational in character, and parameters in any trial $g(x)$ function may be varied to achieve the optimum bound. The problem of end-point solutions in this "classical" limit is not completely resolved. The method can be applied to ground and excited states with little increase in difficulty.

The method will be applied to the field theory problem of a scalar field on a lattice in a later paper. It will be shown to be capable of yielding the exact answer for the vacuum of a massive free field. When applied to a kink-type solution, the quantum effects are shown to be very large when the field tries to vanish. It might be hoped that since this approach leads naturally to classical-like fields, yet quantum effects are not completely neglected, it will provide a better zeroth-order or base problem around which the true quantum effects can be expanded.

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APPENDIX: AN IMPROVED BOUND

In this appendix we will discuss an improvement of the "almost quantum" approximation which still retains the character of a lower bound. Writing $H = H_0 + H'$, where H' is a positive-definite operator, a lower bound to H is obtained by replacing H' by $H'|t\rangle\langle t|H'|t\rangle^{-1}\langle t|H$ for any choice of the trial function t. The ordered eigenvalues of

$$H_s \equiv H_0 + H'|t\rangle\langle t|H'|t\rangle^{-1}\langle t|H'$$

then form lower bounds to the ordered eigenvalues of H. If $|t\rangle$ is an exact wave function, then the corresponding eigenvalue is exact. For H' it is convenient to take, for example, $[p^2 - (h/r^2)]$ with $0 < h < 1$. We now consider a few simple applications of the above.

We start by studying the anharmonic oscillator in one dimension and taking H' to be p^2 which has $h = 0$, the worst possible choice since H' is a maximum. The trial wave function is taken to be $\exp(-\frac{1}{2}ax^2)$. The Schrödinger equation for H_s is

$$(E_s - \lambda x^4)\psi_s = -\frac{J}{a^2}(x^2 - a)e^{-x^2/2a},$$

where $J = \langle t|H'|\psi_s\rangle/\langle t|H'|t\rangle$.

In order that ψ_s be normalizable, it is clear that one must choose $E_s = a^2\lambda$, and hence

$$\psi_s = \frac{J}{E_s}(a^2 + x^2)^{-1}e^{-x^2/2a}.$$

Using these results it is now easy to solve for E_s. The eigenvalue condition can be simplified by rescaling variables:

$$\left(\frac{E_s^3}{\lambda}\right)^{1/2} = \left[\int_0^\infty dy\, e^{-y^2}(1 - y^2)/(1 + y^2)\right]\Big/\left[\int_0^\infty dy\, e^{-y^2}(1 - y^2)\right],$$

so that $E_s = 1.0209\lambda^{1/3}$. This is now within 5% of the exact result.

The same procedure can be carried out for the three-dimensional oscillator $H = \lambda r^4$ with the result $E_s = 3.28$ which is within 15% of the exact result. Of course this method can be used for other levels and potentials, although it becomes algebraically tedious for complicated potentials.

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[3]R. Blankenbecler and J. Fulco, following paper, Phys. Rev. D 17, 514 (1978). The only other attempt we are aware of to derive lower bounds for field theories is R. Pearson, Stanford University Ph. D. thesis (unpublished); Stanford Linear Accelerator Center report, 1975 (unpublished), who used a quite different approach analogous to that of Ref. 2.
[4]M. Einhorn and R. Blankenbecler, Ann. Phys. (N.Y.) 67, 480 (1971).