

Quality of variational trial states

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Various measures for the accuracy of approximate eigenstates of semibounded self-adjoint operators H in quantum theory, derived, e.g., by some variational technique, are scrutinized. In particular, the matrix elements of the commutator of the operator H and (suitably chosen) different operators with respect to degenerate approximate eigenstates of H obtained by the variational methods are proposed as criteria for the accuracy of variational eigenstates. [S1050-2947(99)04112-8]

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I. MOTIVATION

A central element in quantum theory is the solution of eigenvalue problems. However, usually there is no suitable exact solution to which perturbation theory can be applied. A very efficient way to locate the discrete spectrum of some self-adjoint operator H bounded from below is provided by the famous Rayleigh-Ritz variational technique [1]: *If the eigenvalues E_k , $k=0,1,\dots$, of H are ordered according to $E_0 \leq E_1 \leq E_2 \leq \dots$, the first d of them are bounded from above by the d eigenvalues \hat{E}_k , $k=0,1,\dots,d-1$, (ordered by $\hat{E}_0 \leq \hat{E}_1 \leq \dots \leq \hat{E}_{d-1}$) of that operator which is obtained by restricting H to some d -dimensional subspace of the domain of H , i.e., $E_k \leq \hat{E}_k$, $k=0,1,\dots,d-1$.* However, frequently it is not straightforward to quantify how close approximate and exact eigenstates are. Thus, we embark upon a systematic study of the accuracy of the variationally determined eigenstates of H and suitable measures to judge their quality.

II. MEASURES OF THE QUALITY OF TRIAL STATES

Consider some self-adjoint operator H , $H^\dagger = H$, assumed to be bounded from below. Suppressing, for the moment, the index $k=0,1,2,\dots$, let the eigenvalue equation for H ,

$$H|\chi\rangle = E|\chi\rangle, \quad (1)$$

be solved by some (generic) eigenvector $|\chi\rangle$ corresponding to some (real) eigenvalue E . The Rayleigh-Ritz variational technique yields an upper bound \hat{E} on this eigenvalue E as well as, by diagonalization of the relevant characteristic equation, the corresponding vector $|\varphi\rangle$ in the d -dimensional trial space. There exist several (potentially meaningful) measures of the quality of this trial state $|\varphi\rangle$ which immediately come to one's mind:

(1) The trial state $|\varphi\rangle$ is supposed to represent—to a certain degree of accuracy—the approximate solution of the eigenvalue problem defined in Eq. (1). Consequently, a first indicator for the resemblance of $|\varphi\rangle$ with the exact eigenstate $|\chi\rangle$ would be the distance between the expectation value of the operator H with respect to the trial state $|\varphi\rangle$, i.e., between the obtained upper bound $\hat{E} \equiv \langle \varphi | H | \varphi \rangle / \langle \varphi | \varphi \rangle$, and the exact eigenvalue E . However, the precise location of the exact eigenvalue E is usually not known.

(2) The most natural measure for the resemblance of the Hilbert-space vectors $|\varphi\rangle$ and $|\chi\rangle$ under consideration is the overlap

$$S \equiv \frac{\langle \varphi | \chi \rangle}{\sqrt{\langle \varphi | \varphi \rangle \langle \chi | \chi \rangle}} \quad (2)$$

of the trial state $|\varphi\rangle$ with the eigenstate $|\chi\rangle$.

(3) Consider the commutator $[G, H]$ of the operator H under consideration with any other operator G , where the domain of G is assumed to contain the domain of H . Then the expectation value of this commutator with respect to a given eigenstate $|\chi\rangle$ of H vanishes:

$$\langle \chi | [G, H] | \chi \rangle = 0. \quad (3)$$

Hence, choosing different operators G generates a whole class of operators $[G, H]$, each of which may serve to test the quality of a given trial state $|\varphi\rangle$ by evaluating how close the expectation value $\langle \varphi | [G, H] | \varphi \rangle$ with respect to $|\varphi\rangle$ comes to zero. This expectation value vanishes, of course, also if, by accident, the state $|\varphi\rangle$ is an eigenstate of G . However, for a given operator G , after having determined $|\varphi\rangle$, it is straightforward to check for this circumstance, for instance, by inspecting the variance of G with respect to $|\varphi\rangle$; the latter vanishes if $|\varphi\rangle$ is an eigenstate of G . Moreover, it goes without saying that an expectation value $\langle \varphi | [G, H] | \varphi \rangle$ vanishes also if the state $|\varphi\rangle$ is an eigenstate of the commutator $[G, H]$ with eigenvalue 0, or even if the state defined by $[G, H]|\varphi\rangle$ proves to be orthogonal to the state $|\varphi\rangle$.

For any self-adjoint operator G , i.e., $G^\dagger = G$, this commutator is anti-Hermitian, which clearly suggests defining a

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self-adjoint operator $C=C^\dagger$ (on the domain of H) by $[G,H]=iC$. If, for example, G is chosen to be the generator of dilations,

$$G \equiv \frac{1}{2}(\mathbf{x} \cdot \mathbf{p} + \mathbf{p} \cdot \mathbf{x}), \quad (4)$$

relation (3) is precisely the so-called ‘‘master virial theorem’’ introduced in Ref. [2] for a systematic study of (relativistic) virial theorems [3]. In this case, for operators H of the form of some typical Hamiltonian consisting of a momentum-dependent kinetic-energy operator, $T(\mathbf{p})$, and a coordinate-dependent interaction-potential operator, $V(\mathbf{x})$, that is, $H=T(\mathbf{p})+V(\mathbf{x})$, the operator C becomes the ‘‘virial operator’’

$$C = \mathbf{p} \cdot \frac{\partial}{\partial \mathbf{p}} T(\mathbf{p}) - \mathbf{x} \cdot \frac{\partial}{\partial \mathbf{x}} V(\mathbf{x}). \quad (5)$$

The point spectrum (i.e., the set of all eigenvalues) of the dilation generator (4) is empty; in other words, the dilation generator has no Hilbert-space eigenvectors.

III. SPINLESS SALPETER EQUATION

Let us apply the above general considerations to the prototype of all (semi-) relativistic bound-state equations, the ‘‘spinless Salpeter equation,’’ defined by the Hamiltonian (in one-particle form, encompassing also the equal-mass two-particle case [4–7])

$$H = T + V; \quad (6)$$

here T is the relativistic kinetic energy of some particle of mass m and momentum \mathbf{p} ,

$$T = T(\mathbf{p}) \equiv \sqrt{\mathbf{p}^2 + m^2},$$

and $V=V(\mathbf{x})$ is an arbitrary, coordinate-dependent, static interaction potential. The spinless Salpeter equation is then just the eigenvalue equation for the operator H , $H|\chi_k\rangle = E_k|\chi_k\rangle$, $k=0,1,2,\dots$, for the set of eigenvectors $|\chi_k\rangle$ corresponding to the energy eigenvalues E_k . Analytic upper bounds \hat{E}_k on these eigenvalues have been given [4–10].

For the sake of comparison, we focus our interest to central potentials $V(\mathbf{x})=V(r)$, $r \equiv |\mathbf{x}|$. Furthermore, in order to facilitate the numerical treatment of the problem, we only consider the harmonic-oscillator potential

$$V(r) = ar^2, \quad a > 0. \quad (7)$$

The reason for this particular choice is the following: In momentum space, the operator r^2 is represented by the Laplacian with respect to the momentum \mathbf{p} , $r^2 \rightarrow -\Delta_{\mathbf{p}}$, while the kinetic energy T , nonlocal in configuration space, is represented by a multiplication operator. Consequently, exactly for a harmonic-oscillator potential the above semirelativistic Hamiltonian H in its momentum-space representation is equivalent to a nonrelativistic Hamiltonian with some (effective) interaction potential reminiscent of the square root:

$$H = -a\Delta_{\mathbf{p}} + \sqrt{\mathbf{p}^2 + m^2}. \quad (8)$$

The solutions of the corresponding eigenvalue equation may then be found with one of the numerous procedures designed for the treatment of the nonrelativistic Schrödinger equation.

For the harmonic-oscillator potential, it is comparatively easy to get a first idea of the approximate location of the energy levels E_k by entirely analytical considerations:

On the one hand, every eigenvalue E_k is bounded from above by the eigenvalue $E_{k,\text{NR}}$ of the nonrelativistic counterpart of H : $E_k \leq E_{k,\text{NR}}$.

On the other hand, every eigenvalue E_k is bounded from below by the eigenvalue $E_k(m=0)$ of the Hamiltonian H corresponding to vanishing particle mass m : $E_k \geq E_k(m=0)$.

IV. THE ‘‘LAGUERRE’’ TRIAL SPACE

As far as the achieved accuracy of the solutions obtained is concerned, the most crucial step in all variational games of the Rayleigh-Ritz kind is, for the given operator H under consideration, a reasonable definition of the adopted trial subspace of the domain of H .

For spherically symmetric potentials $V(r)$, a very popular choice for the basis states which span the trial space required for the successful application of the variational technique are ‘‘Laguerre’’ trial states, defined in configuration-space representation by [11,9,6,7]

$$\begin{aligned} \psi_{k,\ell m}(\mathbf{x}) = & \sqrt{\frac{(2\mu)^{2\ell+2\beta+1} k!}{\Gamma(2\ell+2\beta+k+1)}} r^{\ell+\beta-1} \\ & \times \exp(-\mu r) L_k^{(2\ell+2\beta)}(2\mu r) \mathcal{Y}_{\ell m}(\Omega_{\mathbf{x}}), \quad (9) \end{aligned}$$

where $L_k^{(\gamma)}(x)$ denote the generalized Laguerre polynomials (for the parameter γ) [12] and $\mathcal{Y}_{\ell m}(\Omega)$ are the spherical harmonics for angular momentum ℓ and its projection m . The trial functions (9) involve two variational parameters, μ (with dimension of mass) and β (dimensionless), which, by the requirement of normalizability of these functions, are subject to the constraints $\mu > 0$ and $2\beta > -1$.

One of the advantages of the trial function (9) is the easy availability of an analytic expression for the corresponding momentum-space representation of these trial states.

For the present investigation, we employ the ‘‘Laguerre’’ trial states defined by Eq. (9), with, for both definiteness and ease of calculation, the variational parameters μ and β kept fixed to the values $\mu = m$ and $\beta = 1$.

V. RATES OF CONVERGENCE OF THE QUALITY MEASURES

Now, let us observe our variational eigenstates $|\varphi\rangle$ approaching the exact eigenstates $|\chi\rangle$ for increasing dimension d of the employed trial space, by comparing the behavior of the various measures for the accuracy of approximate eigenstates discussed in Sec. II.

Without doubt, the only genuine ‘‘point of reference’’ any variational solution to an eigenvalue problem is the corresponding exact solution. The exact solution sought is computed here with the help of the numerical integration procedure developed for the nonrelativistic Schrödinger equation in Ref. [13].

TABLE I. Characterization of the quality of the variational solution of the eigenvalue problem of the semirelativistic Hamiltonian $H = \sqrt{\mathbf{p}^2 + m^2} + V(r)$ with harmonic-oscillator potential $V(r) = ar^2$, for states of radial quantum number $n_r = 0, 1, 2$ and orbital angular momentum $\ell = 0, 1, 2$ (called 1S, 2S, 3S, 1P, and 1D in usual spectroscopic notation). The variational solutions were obtained with the help of our ‘‘Laguerre’’ trial states spanning trial spaces of increasing dimension $d = 1, 2, 25$. We compare the nonrelativistic upper bound E_{NR} and zero-mass lower bound $E(m=0)$ on the energy, the (numerically computed) ‘‘exact’’ energy E , the variational upper bound \hat{E} on this energy, the relative error ε of the upper bound, the deviation from unity σ of the overlap squared of exact and variational eigenstates, the (appropriately normalized) expectation values ν of the virial operator C , and the (normalized) maximum local difference ω of the momentum-space representations of exact and variational eigenstates. The physical parameters are fixed to the values $m = 2$ GeV for the particle mass and $a = 2$ GeV³ for the harmonic-oscillator coupling. A simple entry ‘‘0’’ indicates that the numerical value is closer to 0 than the rounding error.

Quantity	d	State				
		1S	2S	3S	1P	1D
n_r		0	1	2	0	0
ℓ		0	0	0	1	2
E_{NR} (GeV)		4.12132	6.94975	9.77817	5.53553	6.94975
$E(m=0)$ (GeV)		2.94583	5.15049	6.95547	4.23492	5.35234
E (GeV)		3.82493	5.79102	7.48208	4.90145	5.89675
\hat{E} (GeV)	1	4.21624			6.50936	9.77866
	2	3.92759	8.10850		5.24154	7.18242
	25	3.82494	5.79114	7.48290	4.90149	5.89681
ε	1	0.1023			0.3280	0.6583
	2	0.0268	0.4002		0.0694	0.2180
	25	0	0	0.0001	0	0
σ	1	0.09618			0.36144	0.65587
	2	0.02375	0.43693		0.09001	0.34398
	25	0	0	0.00008	0	0
ν	1	-0.6120			-0.8328	-0.9074
	2	+0.0308	-0.8666		-0.5103	-0.7483
	25	0	-0.0001	+0.0001	0	0
ω	1	+0.9277			+0.7541	+1.0578
	2	-0.00754	+2.4577		+0.3598	+0.7262
	25	+0.00003	-0.0017	+0.0002	+0.0004	+0.0003

Table I confronts, for the ground state and the lowest radial and orbital excitations, the approximate solutions as calculated with the help of the Rayleigh-Ritz variational technique for ‘‘Laguerre’’ trial subspaces of the domain of H of increasing dimension d with the exact solutions of the eigenvalue problem for the semirelativistic Hamiltonian (6) with a central interaction potential of the harmonic-oscillator form (7). First of all, as discussed in Sec. III, the exact position of any eigenvalue E of our Hamiltonian H is confined to a range defined by the nonrelativistic upper bound E_{NR} and the zero-mass lower bound $E(m=0)$ on this energy eigenvalue E . There are several quantities which may participate in a competition for ‘‘the best or most reasonable measure of quality:’’

(1) The relative error $\varepsilon \equiv (\hat{E} - E)/E$ of every upper bound \hat{E} on the exact energy eigenvalue E is, by definition, always non-negative, i.e., $\varepsilon \geq 0$.

(2) The deviation from unity, σ , of the modulus squared of the overlap S of exact and variational eigenstates defined in Eq. (2), $\sigma \equiv 1 - |S|^2$, is necessarily confined to the range $0 \leq \sigma \leq 1$.

(3) The use of the expectation values of the commutators $[G, H]$ with respect to the variational eigenstates $|\varphi\rangle$ is illus-

trated for the particular example of the dilation generator G defined in Eq. (4), by considering (suitably normalized) expectation values $\langle \varphi | C | \varphi \rangle$ of the virial operator C given in Eq. (5):

$$\nu \equiv \frac{\langle \varphi | C | \varphi \rangle}{\langle \varphi | \mathbf{x} \cdot \frac{\partial}{\partial \mathbf{x}} V(\mathbf{x}) | \varphi \rangle} = \frac{\langle \varphi | \mathbf{p} \cdot \frac{\partial}{\partial \mathbf{p}} T(\mathbf{p}) | \varphi \rangle}{\langle \varphi | \mathbf{x} \cdot \frac{\partial}{\partial \mathbf{x}} V(\mathbf{x}) | \varphi \rangle} - 1.$$

(4) Finally, the normalized maximum difference of the normalized momentum-space representations $\tilde{\varphi}(\mathbf{p})$ and $\tilde{\chi}(\mathbf{p})$ of the variational eigenstate $|\varphi\rangle$ and exact eigenstate $|\chi\rangle$, respectively, i.e., the maximum pointwise relative error in momentum space, $\omega \equiv \max_{\mathbf{p}} [|\tilde{\varphi}(\mathbf{p}) - \tilde{\chi}(\mathbf{p})|] / \max_{\mathbf{p}} \tilde{\chi}(\mathbf{p})$, is listed.

Note that the only measure for the accuracy of approximate eigenstates $|\varphi\rangle$ which does not require any information other than the one provided by the variational technique is ν , i.e., the (normalized) expectation values of the commutator $[G, H]$ with respect to $|\varphi\rangle$. Inspection of Table I reveals that ν represents indeed a sensitive measure of quality: for in-

creasing trial-space dimension d it converges to zero at roughly the same rate as both energy and overlap error, ε and σ , but makes more sense than a pointwise error like ω .

VI. SUMMARY AND CONCLUSIONS

Various measures for the accuracy of approximate eigenstates of arbitrary (self-adjoint, semibounded) operators H have been studied. The vanishing of the expectation values of the commutator of H and any other well-defined operator,

taken with respect to the approximate eigenstates, provides a useful set of criteria for estimating the significance of the variational solution. This has been illustrated by considering the commutator of the Hamiltonian of the spinless Salpeter equation and the generator of dilations.

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