Variational estimates of the energy of excited states

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The energies of excited states for two- and three-particle systems with arbitrary blocking potential are calculated within the framework of a naive variational approach. The uncertainty in the calculation of the energy of the lower excited states is comparable with the uncertainty in the calculation of the energy of the ground state and in all cases is much less than 1%. The energy of the highly excited states is found with the help of a variational approach in the classical limit: the true functional dependence on the quantum numbers is reproduced with errors of the order of 1% for the numerical coefficients of the asymptotic expansion. The classical variational principle for the time-averaged Hamiltonian for periodic motions with fixed action is discussed. © *1995 American Institute of Physics.*

1. INTRODUCTION

Three-body systems are of great interest for baryon physics. The spectrum of baryon resonances has been successfully reproduced within the framework of the quark model with interaction potentials "derivable" from quantum chromodynamics (QCD).[1] Parallel efforts have been made to solve the inverse problem and, so to speak, "derive" the QCD potential from the spectroscopic data. Remarkable successes in this direction were achieved for systems of quarkonium type,[2,3] with somewhat more modest results for baryons.[4] In the present paper we will follow the inverse approach and develop approximate methods for calculating the energy with the goal of analyzing the energy spectrum of three-particle systems. A detailed and excellent review of numerous regular exact calculational methods for three-body systems was published recently by Richard.[4] In the present paper we claim to achieve a calculational accuracy on the order of 1%, which for masses of the order of $2\cdot 10^3$ MeV amounts to 20 MeV—an accuracy, from our point of view, entirely suitable for the physics of resonances. The level of mathematical rigor which we have adopted is customary for theoretical physics and more like the level of accuracy of Ref. 2 than of Ref. 3.

The method we develop and use is a naive generalization of the customary variational procedure used to calculate the ground state energy. We devote the following section to a discussion of this method in the simple case of a one-dimensional system. Next we examine a number of details and discuss the mathematical principles lying at the basis of the method, and then turn to three-dimensional problems (Sec. 3). In Sec. 4 we consider the three-body problem and compare our simple results with accurate numerical calculations of other authors. Having shown that the method works, we make an effort to apply it to an analysis of the experimental data on baryon resonances. (References to the voluminous literature are provided in the corresponding sections, and not in this brief introduction.)

Let us indicate the main idea of the paper. According to the Variational Principle,[6] an extremum of the integral $\langle\Psi|H|\Psi\rangle$ for variations of the normalized wavefunctions Ψ is reached at the eigenfunctions of the operator H. The lowest state of H determines the absolute minimum of the integral, the remaining eigenstates correspond to local extrema in Hilbert space. Thus, the eigenvalue of the integral can be estimated if you find yourself at the right place in Hilbert space. But how to determine the "right" place?

We choose an orthonormal set of eigenfunctions (e.g., of the harmonic oscillator) in which we can vary the scale. If the first function of the set (after choosing the scale) yields a good approximation to the lowest state, we assume that the second function of this orthonormal set also gives a good approximation to the second eigenvalue, etc. We will convince ourselves by way of numerous examples that his crude idea works. More precisely, the relative error grows slowly with increasing energy. However, for lower excitations variational estimates turn out to be just as useful as for the ground state. We will discuss the inaccuracy of the method in more detail in Sec. 2 by way of examples. It is interesting that the energy levels in the asymptotic limit of large quantum numbers n can be obtained by using variational estimates for classical quantities, and these asymptotic formulas give very good accuracy even for small n.

2. A SIMPLE EXAMPLE: ONE-DIMENSIONAL LINEAR POTENTIAL

Let us consider the energy levels for the Schrödinger equation with a linear potential (throughout this paper we set $\hbar=1$):

$$H\Psi_n(x)=\left[-\frac{d^2}{dx^2}+x\right]\Psi_n(x)=E_n\Psi_n(x), \qquad (2.1)$$

where $0\leqslant x\leqslant\infty$, and the boundary conditions are chosen in the form $\Psi(0)=\Psi(\infty)=0$. This is the well-known quantum-mechanical problem of motion under the action of a constant force.[2,3]

The eigenvalues E_n of Eq. (2.1) are given by the zeros of the Airy function and the eigenfunctions $\Psi_n(x)$ coincide with the Airy functions themselves. The zeros and values of the Airy functions are tabulated (see, e.g., Ref. 5). In Table I we give a few of the first eigenvalues. In order to begin and decide on our notation, we calculate the energy of the ground state by the variational method, using as our trial function the

TABLE I. Linear potential in one dimension.

n	$2n+1$	$\bar{\omega}_{2n+1}$	$E_n^v(\bar{\omega})$	E_n^{exact}	ΔE_n	δE_n	$\Delta E_n/(E_{n+1}-E_n)$
0	1	0.52106	2.3448	2.3381	0.0067	0.29%	+0.39%
1	3	0.3881	4.0752	4.0879	−0.0127	−0.31%	−0.89%
2	5	0.3332	5.4978	5.5206	−0.0228	−0.41%	−1.81%
3	7	0.3003	6.7565	6.7867	−0.0302	−0.44%	−2.62%
4	9	0.2775	7.9076	7.9441	−0.0365	−0.46%	−3.40%
5	11	0.2603	8.9804	9.0226	−0.0462	−0.47%	−4.54%

wave function of the harmonic oscillator. It is more convenient, instead of Eq. (2.1), to consider motion over the entire axis $-\infty<x<\infty$ with the potential $V(x)=|x|$. As our unperturbed Hamiltonian we choose

$$H^{(0)}(\omega)=-\frac{d^2}{dx^2}+\omega^2x^2, \tag{2.2}$$

the obvious form associated with the standard harmonic oscillator. Then as our trial function for the ground state E_0 in problem (2.1), we choose the wave function of the first excited state of problem (2.2) since it is precisely this wave function that corresponds to the lowest state with a zero of the wave function at $x=0$:

$$\Psi_1^{(0)}(\omega,x)=\left(\frac{\omega}{\pi}\right)^{1/4}\sqrt{2\omega}x\,\exp\left(-\frac{\omega x^2}{2}\right). \tag{2.3}$$

We calculate the mean value of the Hamiltonian with the trial function (2.3)

$$E_0(\omega)=\langle\Psi_1^{(0)}|H|\Psi_1^{(0)}\rangle=\frac{3}{2}\,\omega+\frac{2}{\sqrt{\pi\omega}}, \tag{2.4}$$

where the first term comes from the kinetic energy, and the second from the potential energy $|x|$. Taking the minimum of $E_0(\omega)$ over the frequency ω, we find

$$\bar{\omega}_1=\left(\frac{4}{9\pi}\right)^{1/3}\simeq 0.52106 \tag{2.5}$$

and the corresponding minimum for E_0:

$$E_0^v(\bar{\omega}_1)=\frac{9}{2}\,\bar{\omega}_1=\frac{9}{2}\left(\frac{4}{9\pi}\right)^{1/3}\simeq 2.3448, \tag{2.6}$$

in good agreement with the first zero of the Airy function, the accurate value of the energy being $E_0\simeq 2.3381$. Thus we have obtained a good approximation both for the lowest energy (2.6) and for the wavefunction $\Psi_1^{(0)}(\bar{\omega},x)$. It is reasonable to assume that if Ψ_1 gives such a good value for E_0, Ψ_3 should also give a good approximation for E_1. Therefore we take the following eigenfunction of $H^{(0)}(\omega)$, which satisfies the boundary condition $\Psi_{(0)}=0$:

$$\Psi_3^{(0)}(\omega,x)=\left(\frac{\omega}{\pi}\right)^{1/4}\frac{1}{\sqrt{3}}\,[2(\sqrt{\omega}x)^3-3(\sqrt{\omega}x)] \times\exp\left(-\frac{\omega x^2}{2}\right). \tag{2.7}$$

The mean value of the Hamiltonian H for the trial function (2.7) is

$$E_1(\omega)=\frac{7}{2}\,\omega+\frac{3}{\sqrt{\pi\omega}}\cdot \tag{2.8}$$

Taking the minimum of $E_1(\omega)$ over ω, we obtain $\bar{\omega}_3$,

$$\bar{\omega}_3=\left(\frac{9}{49\pi}\right)^{1/3}\simeq 0.3881, \tag{2.9}$$

and the mean value of the energy E_1^v,

$$E_1^v(\bar{\omega}_3)=\frac{21}{2}\,\bar{\omega}_3=\frac{21}{2}\left(\frac{9}{49\pi}\right)^{1/3}\simeq 4.0752, \tag{2.10}$$

which (as we assumed) is found to be in good agreement with the position of the second zero of the Airy function, i.e., with the accurate value of the energy $E_1\simeq 4.0879$, although it is a little (0.31%) smaller than it. Note that $\bar{\omega}_3\neq\bar{\omega}_1$ and therefore the trial functions are not orthogonal. We can calculate the mean energy over the nth odd state of the oscillator:

$$E_n(\omega)=\left(2n+\frac{3}{2}\right)\omega+\frac{(2n+1)!}{2^{2n-1}(n!)^2\sqrt{\pi\omega}},$$

and analogously obtain a variational value of the energy

$$E_n^v(\bar{\omega}_{2n+1})=\frac{3}{2}\,(4n+3)^{1/3}\left[\frac{(2n+1)!}{2^{2n-1}(n!)^2\sqrt{\pi}}\right]^{2/3}. \tag{2.11}$$

The variational values $E_n^v(\bar{\omega}_{2n+1})$ are given in Table I for the first six states, where they are compared with the exact values E_n^{exact}. From the table it is immediately apparent that the difference $\Delta E_n = E_n^v - E_n^{\mathrm{exact}}$ grows slowly in absolute value with increasing n, roughly with the same rate as E_n, so that the relative error δE_n remains approximately constant between $n=0$ and $n=5$. Note also that ΔE_n is negative for the excited states.

The asymptotic value of E_n^v is

$$\lim_{n\to\infty} E_n^v=6\left(\frac{n+3/4}{\pi}\right)^{2/3}\simeq 2.7972\left(n+\frac{3}{4}\right)^{2/3}, \tag{2.12}$$

which is approximately 0.5% lower than the the asymptotic value calculated with the help of the quasiclassical WKB approximation

$$E_n^{WKB}=\left[\frac{3\pi}{2}\left(n+\frac{3}{4}\right)\right]^{2/3}\simeq 2.8108\left(n+\frac{3}{4}\right)^{2/3}. \tag{2.13}$$

Thus, in absolute value the variational estimates differ from the true values by not more than 0.5%. It should be borne in mind, however, that the frequency of the levels grow with increasing n. Therefore for large enough quantum numbers,

TABLE II. Variational values for the mean values of the operators.

n	$\langle H^2\rangle$	$E_n^2(\bar\omega)$	$\langle H^2\rangle/E_n^2(\bar\omega)$	$\langle x^2\rangle$	$\langle x^2\rangle_{exact}$	$\delta\langle x^2\rangle$
0	5.5259	5.4981	1.0050	2.8787	2.9156	−1.27%
1	16.7630	16.6073	1.0094	9.0183	8.9125	+1.19%
2	30.5419	30.2258	1.0104	16.5066	16.2544	+1.55%
3	46.1442	46.0593	1.0108	24.9750	24.5649	+1.67%
4	63.2207	62.5301	1.0110	34.239	33.658	+1.73%
5	81.5416	80.6476	1.0111	44.179	43.417	+1.75%

TABLE III. Probability of overlap with the true eigenstates (in %).

n	P_0	P_1	P_2	P_3	P_4	P_5	ΣP_n
0	99.82	0.017	0.101	0.041	0.013	0.004	99.996
1	2.52	96.00	0.811	0.556	0.092	0.016	99.995
2	0.74	5.13	89.50	3.43	1.09	0.101	99.39
3	0.235	1.79	7.82	80.75	7.78	1.65	100.03
4	0.09	0.62	3.15	10.22	70.35	13.69	98.12
5	0.04	0.25	1.20	4.72	12.06	58.95	77.22

between the exact value E_n^{exact} and the variational value E_n^v it is possible to locate many levels with other n. The critical value of the number for which E_n^v is closer to its first neighbor $E_{n\pm 1}^{\text{exact}}$ than to E_n^{exact} is $n_{\text{cr}}\simeq 137$. This means that the variational estimates are reasonable (in this sense), say, for $n\lesssim 20$.

The asymptotic limit (2.12) can be obtained, of course, from the general expression (2.11) if we make use of Stirling's formula for the factorial. A more beautiful and direct path, which allows us to do without expression (2.11), is to apply the variational method in the quasiclassical limit. Indeed, for the classical trajectory $x(t)=A\sin\omega t$, the energy is equal to $E=A^2\omega^2/2=2(n+1/2)\omega$. Hence it is possible to determine the coefficient A and thereby find the mean value of $|x|$

$$\langle |x|\rangle=\frac{2A}{\pi}=\frac{4}{\pi}\sqrt{\frac{n+1/2}{\omega}},$$

and the mean value of the Hamiltonian (2.1)

$$\langle H\rangle=\left(n+\frac{1}{2}\right)\omega+\frac{4}{\pi}\sqrt{\frac{n+1/2}{\omega}}. \tag{2.14}$$

The extremum of $\langle H\rangle$ determines $\bar\omega_n$ and the asymptotic behavior of E_n^v (2.12). (Recall that n are all odd integers.)

Although the variational energies are very close to the true eigenvalues, it is also useful to understand how close the variational states $\Psi_{2n+1}^{(0)}(\bar\omega)$ are to the eigenfunctions of the Hamiltonian (2.1). With this goal in mind, let us calculate the mean value of the square of the Hamiltonian H^2 for the variational states of the oscillator and determine the difference $\langle H^2\rangle-\langle H\rangle^2$. The smaller this difference, the closer the variational functions will be to the corresponding eigenfunctions. The results of these calculations are presented in Table II, from which it can be seen that the ratio $\langle H^2\rangle/\langle H\rangle^2$ grows slowly with n. We have found that in the limit, $(\langle H^2\rangle-E_n^2)/E_n^2\simeq 0.011$. Hence it is clear that the expansion of the variational function over the eigenstates is quite narrow. We can also calculate numerically the overlap integral of the variational functions for $\omega_n=\bar\omega_n$ with the correspondingly normalized Airy functions. The squares of these amplitudes are the corresponding probabilities. Their values are given in Table III. For the trial ground state the probability of being in the true ground state is greater than 99%.

The corresponding probabilities for higher states are lower. Thus, for the third excited state the probability of being in the true ($n=3$) state is equal to only 80%, but the distribution over "foreign" states turns out to be symmetric: $P_2\simeq P_4\simeq 7.8\%$ and $P_1\simeq P_5\simeq 1.75\%$, so that the "mean" values turn out to be in the right place. The table of probabilities can be additionally checked by calculating the matrix elements of H and H^2 from the expansion coefficients and comparing the results with Tables I and II. It can be seen that the energy and its square are calculated much more accurately than the wavefunctions themselves. Other operators, say x^2 (its matrix elements are given in Table II), can also be calculated to high accuracy (errors less than 2%). The probability distributions in Table III prove that the variational estimates of the energies actually correspond to the states they are assigned to, i.e., E_3^v really is the energy of the fourth state (we start with $n=0$), etc. Of course, it is possible to calculate the probability distributions only in the simplest cases (as in ours) for which the wavefunctions are known. Therefore it is useful to have an "internal" criterion for the accuracy of the calculations.

We will assume that the exact eigenvalues are unknown to us. How can we estimate the error of the variational calculations? A simple way of doing it is to consider the variational values as energy values in the first order of perturbation theory with respect to the unperturbed Hamiltonian $H^{(0)}(\bar\omega_n)$ for fixed $\bar\omega$ (for given energy level). Further, we can estimate the contribution of the second order in perturbation theory and take this as an estimate of the inaccuracy in the calculation of the energy. We illustrate this calculation in the instance of the ground state E_0 and the first excitation E_1. For the ground state we have

$$\Delta E_0^{(2)}=-\sum_{n=1}\frac{|\langle 2n+1|V|1\rangle|^2}{2n\bar\omega},$$

where $V=|x|-\omega^2x^2$,

$$\langle 3|V|1\rangle=\frac{0.4607}{\sqrt{\omega}}-1.2247\omega,$$

$$\langle 5|V|1\rangle=-\frac{0.103}{\sqrt{\omega}},\quad \langle 7|V|1\rangle=-\frac{0.0477}{\sqrt{\omega}}.$$

Thus,

$$\Delta E_0^{(2)}=-\frac{0}{2\bar\omega}-\frac{(0.1427)^2}{4\bar\omega}-\frac{(0.061)^2}{6\bar\omega}-\ldots\simeq -0.011.$$

Note that the second-order correction to the ground state due to mixing with the first excited state disappears when $\omega=\bar\omega=0.521$. This is an absolutely general result for oscillator trial functions—for any interaction the first excited state does not mix into the ground state for the extreme value of the frequency $\bar\omega$. The estimate of $\Delta E_0^{(2)}$ is of the same magnitude as the error in the calculation of the energy of the ground state: the corrected value $(2.3448-0.011)\simeq 2.3338$ now lies a little bit below the true value. Let us now repeat this same calculation for the first excited state (for which $\omega=\bar{\omega}_3=0.388$):

$$\Delta E_1^{(2)}=-\sum_n{}' \frac{|\langle 2n+1|V|3\rangle|^2}{(2n-2)\bar{\omega}},$$

$$\langle 5|V|3\rangle=\frac{0.6308}{\sqrt{\omega}}-2.2361\,\omega,$$

$$\langle 7|V|3\rangle=\frac{0.1363}{\sqrt{\omega}}.$$

Substituting these matrix elements, we obtain

$$\Delta E_1^{(2)}=\frac{(0.2644)^2}{2\bar{\omega}}-\frac{(0.1451)^2}{2\bar{\omega}}-\frac{(0.2188)^2}{4\bar{\omega}}-\frac{(0.099)^2}{6\bar{\omega}}-\ldots\simeq 0.0900-0.0271-0.0308-0.0042\simeq 0.0279.$$

Again the value obtained is numerically somewhat greater than the real error of calculation of E_1, but this procedure still gives an "internal" estimate of the accuracy of the method. The smallness of the ratio $\Delta E_1^{(2)}/E_1(\bar{\omega})$ confirms that the unperturbed Hamiltonian $H^{(0)}(\bar{\omega})$ is an appropriate starting point for the perturbation theory and that the first order of this theory already gives a good approximation to the exact answer.

3. DISCUSSION OF THE METHOD

In the Introduction it was noted that the proposed method is based on the Variational Principle. This principle states that the eigenvalues of the operator H are extrema of the corresponding integral for certain types of variations. However, there exists a set of particular questions lying outside this general statement.

One of these questions, which at once comes to mind, is, why does the second function $\Psi_2^{(0)}$ in a "arbitrary" orthonormal set of functions estimate precisely the second eigenvalue of the Hamiltonian H with exact wavefunction Ψ_2? Clearly, if $\Psi_2^{(0)}$ is orthogonal to the true ground state Ψ_1, then the variational estimate should give an upper bound on the true energy E_2. However, although $\Psi_2^{(0)}$ is orthogonal only to $\Psi_1^{(0)}$, the minimax theorem[7,3] asserts that the true energy E_2 is an upper bound on all minima of mean values of H if we vary $\Psi_1^{(0)}$ over the entire Hilbert space. The upper bound is attained at $\Psi_1^{(0)}=\Psi_1$. Thus, even the mean value $E_2^{(0)}(\bar{\omega})$ possesses extremal properties and in general should be lower than the true eigenvalue E_2. In order to satisfy the conditions of the minimax theorem, it is necessary to vary $\Psi_2^{(0)}$ over a wider range than we are doing here (by varying the scale of ω), for example, by taking arbitrary linear combinations with $\Psi_3^{(0)}$, $\Psi_4^{(0)}$,..., etc. However, even the incomplete procedure which we follow can give a reasonable approximation. Why the errors are so small is the question here, or, more accurately, it is a matter of choosing a good orthonormal starting system. In the example of the foregoing section we showed that for weakly excited states (small n) the best variational wavefunctions have a small "admixture" from neighboring states and, moreover, this admixture is symmetric, so that the mean values turn out to be close to the right place. Our experiment convinces us that errors in the calculation of the excited states are very similar to errors in the calculation of the ground state. A peculiarity of the problems considered so far is that we have limited the discussion to confinement potentials without complicated structure. In these examples the variational procedure for any level n reduces to choosing the right scale of the wavefunction by varying only ω—the scale of the starting potential. However, this is no guarantee that the orthonormal set of wavefunctions thus chosen will be successful. In each case it is necessary to try and see. As was explained in the foregoing section, we always have an "internal" criterion for estimating the errors, which consists namely of calculating in second-order perturbation theory. (Note that this step requires much more work than calculating the variational energies themselves.)

A separate question of interest touches on quasiclassical calculations when we apply the variational method directly in the classical region in order to reproduce the asymptotic limit of the general variational formulas. These calculations assume the existence of a variational principle for $\langle H\rangle$ in classical mechanics. We have discovered that such a principle actually exists for variations of $\langle H\rangle$ with respect to periodic trial motions that conserve the reduced action. The period changes, but the action remains constant. The true energy is an extremum of $\langle H\rangle$. The quantum version of this variational principle was used by Schrödinger himself in the derivation of his equation. This principle extends the principle of Maupertuis, which was formulated for trial motions with constant energy, to trial motions with constant action. The derivation is given in Appendix A. (A particular version of this classical principle was postulated by Van Vleck in 1923.[7])

Let us turn now to the literature, where our knowledge is obviously incomplete. In a very remote sense our procedure is reminiscent of the "Principle of Least Sensitivity" of Stevenson[9] (introduced in a different context.) The frequency ω is an artificial quantity, generally speaking, not bearing any relation to the Hamiltonian H. If we calculate all orders of the perturbation theory for $E_n(\omega)$, then the answer ceases to depend on the initial value of ω. Thus, choosing the value of $\bar{\omega}$ such that $dE(\bar{\omega})/d\omega=0$, we are already guaranteed that $E(\bar{\omega})$ will be insensitive to first order to this value, and in this way we make a good choice.

Our procedure also bears some relation to the work of Mathews *et al.*[10] on the quadratic potential, in which they used the harmonic oscillator basis and chose the frequencies ω_n for each level n such that the contributions of the nearest states $n\pm 2$ to the energy cancelled in second-order perturbation theory. Without a doubt, the procedure is more cumbersome, because it requires one to calculate the nondiagonal matrix elements; however, the idea of using different ω_n for different states n is, in essence, very similar. (In our procedure there is a partial cancellation of the $n\pm 2$ contributions for the excited states and exact cancellation for the ground state.)

It is interesting to know when the variational method can lead to unreasonable results for the excited states. We have examined one simple case, which possibly gives some indications. We used the wavefunctions of the three-dimensional harmonic oscillator in order to estimate the energy of the first excited state (the $2s$ state) of the hydrogen atom: we found that $E_2 \simeq -0.126$, which is very close to the exact value $E_2 = -1/8$ (in atomic units). Since the Coulomb wavefunctions are well known, it is not difficult to calculate the overlap integrals. As a result we found that the trial function has a probability of 1% of being in the right ($2s$) state. Thus, a good approximation for the energy arises as a result of very close cancellations. Moreover, estimates of the second-order terms of the perturbation theory show that each of them is quite large and the result is unstable to these corrections. We suspect that the lack of success of the method in the case of potentials of the form r^p with negative p is connected with the more singular behavior of the potential at the origin $r=0$ in comparison with the trial Hamiltonian, and also with the existence of a continuous spectrum.

Three-dimensional example

The eigenvalues of the energy found for one-dimensional motion with a linear potential are also suitable for s-wave bound states of systems in three variables.[5] Let us now consider the three-dimensional problem in more detail. The wave equation has the form

$$[-\nabla^2 + r]\Psi_{nlm}(\mathbf{r}) = E_{nl}\Psi_{nlm}(\mathbf{r}). \tag{3.1}$$

We will calculate E_{nl} as the mean value of the Hamiltonian $(-\nabla^2 + r)$ from the eigenfunctions of the harmonic oscillator $(-\nabla^2 + \omega^2 r^2)$ in three dimensions. The energy of the oscillator is equal to $2(2n+l+3/2)\omega$, and the mean value for the kinetic energy, according to the virial theorem, is equal to $(2n+l+3/2)\omega$. It remains to calculate the matrix element of r over the oscillator wavefunctions $\Psi^{(0)}_{nlm}$. We have not found a simple, compact expression for the general expression for this matrix element. Let us therefore consider different limiting cases. For $n=0$ we find

$$E^v(0,l) = \frac{3}{2}(2l+3)^{1/3}\left[\frac{\Gamma(2+l)}{\Gamma\left(\frac{3}{2}+l\right)}\right]^{2/3}, \tag{3.2}$$

for $n=1$

$$E^v(1,l) = \frac{3}{2}(2l+7)^{1/3}\left[\left(l+\frac{9}{4}\right)\frac{\Gamma(2+l)}{\Gamma\left(\frac{3}{2}+l\right)}\right]^{2/3}, \tag{3.3}$$

and for $n=2$

$$E^v(2,l) = \frac{3}{2}(2l+11)^{1/3}\left[\frac{(l^2+\frac{11}{2}l+\frac{225}{32})}{(l+\frac{3}{2})(l+\frac{5}{2})}\frac{\Gamma(2+l)}{\Gamma(\frac{3}{2}+l)}\right]^{2/3}. \tag{3.4}$$

Table IV compares these formulas with the "exact" eigenvalues calculated by numerical integration of the radial equation. It is clear from the table that the variational values are in good agreement with the exact values, and the accuracy of agreement improves as l increases. We also obtained (numerically) the WKB approximations for these eigenvalues and discovered that they differ from the "exact" values more than do the variational values. Thus, for $n=2$, $l=3$, the WKB approximation gives $E_{2,3} = 7.4834$, which corresponds to an error of $\approx 0.28\%$, whereas the variational value 7.5007 differs from the true value by only 0.05%.

TABLE IV. Variational values for a linear potential in three dimensions.

nl	E^v_{nl}	E^{exact}_{nl}	$\Delta E^v/E$	E_{nl} (3.6)
00	2.3448	2.3381	0.29 %	2.3090
01	3.3678	3.3612	0.20%	3.3164
02	4.2544	4.2482	0.15%	4.3051
03	5.0569	5.0509	0.12%	5.2863
10	4.0752	4.0879	−0.31%	4.0620
11	4.8797	4.8844	−0.10%	4.8282
12	5.6297	5.6297	−0.00%	5.5839
13	6.3350	6.3321	+0.05%	6.3332
20	5.4978	5.5206	−0.41%	5.4904
21	6.1928	6.2076	−0.24%	6.1515
22	6.8603	6.8689	−0.12%	6.8057
23	7.5007	7.5046	−0.05%	7.4550

For the first two s-wave states we compared square of the modulus of the wave functions at zero $|\Psi(0)|^2$ for the true and the variational wave functions. For Hamiltonian (3.1) the quantity $|\Psi(0)|^2$ for all s-states is equal to $(4\pi)^{-1} = 0.0795$, whereas for the harmonic oscillator, for the ground state we have $|\Psi_{1s}(0)|^2 = 2/3\pi^2 \simeq 0.0675$, and for the first excited state we have $|\Psi_{2s}(0)|^2 = 9/14\pi^2 \simeq 0.0651$. Errors of 15–18% in the wave function are in full accord with small errors in the energy since the latter are quadratic in the errors in the wave functions.

We also obtained an asymptotic formula for the energy levels of Hamiltonian (3.1) with the help of variational calculations in the quasiclassical region. In the limit of small l, $l \ll n$, we have

$$\langle r \rangle_{nl} = \frac{1}{\pi\sqrt{\omega}}\left[4\sqrt{n+\frac{3}{4}} + \frac{l}{\sqrt{n+\frac{3}{4}}}\right]. \tag{3.5}$$

Accordingly,

$$E_{nl} = 6\left(n+\frac{l}{2}+\frac{3}{4}\right)^{1/3}\left[\frac{1}{\pi}\sqrt{n+\frac{3}{4}} + \frac{l}{4\pi\sqrt{n+\frac{3}{4}}}\right]^{2/3}. \tag{3.6}$$

These calculations are valid in the limit $l \ll n$, when the centrifugal potential is responsible for a weak perturbation. However, formula (3.6) works very well even for small n (errors of the order of $\sim 1\%$, as can be seen from Table I). For $l=0$, expression (3.6) reduces to expression (2.12).

4. THE THREE-BODY CASE

In this section we will consider how the variational method works in the case of the three-body problem with pairwise interactions. Let all the particles have the same mass $m=1$. Then the Hamiltonian has the form

$$H=\frac{1}{2}\sum_{1}^{3}\mathbf{p}_i^2+\frac{1}{2}\sum_{i<j}r_{ij}^p, \tag{4.1}$$

where $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$, and the power $p>0$. Let us compare our results with the numerical calculations presented in Richard's review[5] for $p=1$ and in Refs. 5 and 11 for $p=0.1$. Eliminating center-of-mass motion and introducing the Jacobi coordinates

$$\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3=0,\quad \sqrt{2}\boldsymbol{\rho}=\mathbf{r}_1-\mathbf{r}_2,\quad \sqrt{6}\boldsymbol{\lambda}=\mathbf{r}_1+\mathbf{r}_2-2\mathbf{r}_3,$$

we obtain a Hamiltonian that depends only on $\boldsymbol{\rho}$ and $\boldsymbol{\lambda}$. As our zeroth approximation, let us now consider the three-particle harmonic oscillator with Hamiltonian $H^{(0)}(\omega)$:

$$H^{(0)}(\omega)=\tfrac{1}{2}(\mathbf{p}_\rho^2+\mathbf{p}_\lambda^2)+\tfrac{1}{2}\omega^2(\boldsymbol{\rho}^2+\boldsymbol{\lambda}^2), \tag{4.2}$$

which corresponds to Hamiltonian (4.1) for $p=2$ ($\omega^2=3$). The energy eigenvalues $H^{(0)}(\omega)$ are equal to $E_N=(N+3)\omega$ and, with the exception of the ground state, are highly degenerate. The eigenstates can be classified according to the eigenvalues of the angular momentum $\mathbf{L}^2$ and L_z and according to the permutation symmetry of the indices 1, 2, 3 of the "initial" particles. For low excitations these quantum numbers are sufficient for complete identification of the quantum states; however, for large N the states with fixed L and L_z and permutation symmetry can still be degenerate.[5,12] We will be interested in the ground state, the lower P and D waves ($L=1,2$), and the first excitation with $L=0$. These states are completely symmetric or antisymmetric under permutation. We start by applying the variational method to the ground state, where the calculational procedure and the result are well known.

For completely symmetric (or antisymmetric) states Ψ^s, the mean value of the potential energy can be written in the simple form

$$\langle V\rangle_s=\left\langle\Psi^s\left|\frac{1}{2}\sum_{i<j}r_{ij}^p\right|\Psi^s\right\rangle=\frac{3}{2}\langle\Psi^s|r_{12}^p|\Psi^s\rangle, \tag{4.3}$$

i.e., in terms of the mean value of the interparticle distance of one pair r_{12}, and in Jacobi coordinates

$$\boldsymbol{\rho}=\frac{1}{\sqrt{2}}(\mathbf{r}_1-\mathbf{r}_2), \tag{4.4}$$

it has the form

$$\langle V\rangle_s=\frac{3\cdot 2^{p/2}}{2}\langle\Psi^s|\rho^p|\Psi^s\rangle. \tag{4.5}$$

Here $\rho=|\boldsymbol{\rho}|$. Thus, the mean value of the Hamiltonian requires in the given case that we calculate the matrix elements of only one coordinate. The kinetic energy obviously coincides with the kinetic energy for the harmonic oscillator and according to the virial theorem is equal to half the total energy E_N. Recall that the wavefunction of the ground state $H^{(0)}$ is

$$\Psi_{00}^{(0)}=\frac{\exp[-(\rho^2+\lambda^2)/2]}{\pi^{3/2}} \tag{4.6}$$

(we set $\omega=1$; the dependence on ω in the final answer can be easily recovered from dimensionality). Then

$$\langle\Psi_{00}|V|\Psi_{00}\rangle=\frac{3\cdot 2^{p/2}}{2\pi^3}\int d^3p\,d^3\lambda\exp[-(\rho^2+\lambda^2)]\rho^p$$

$$=\frac{3\cdot 2^{p/2}}{\sqrt{2}}\Gamma\left(\frac{3+p}{2}\right) \tag{4.7}$$

and therefore the mean value of $H(\omega)$ in the ground state is

$$E_{00}(\omega)=\frac{3}{2}\omega+\frac{3}{\sqrt{\pi}}\left(\frac{2}{\omega}\right)^{p/2}\Gamma\left(\frac{3+p}{2}\right) \tag{4.8}$$

(we have reconstructed the dependence on ω). The variational procedure leads to the expression

$$E_{00}^v=3\left(\frac{2+p}{p}\right)\left[\frac{p}{2\sqrt{\pi}}\Gamma\left(\frac{3+p}{2}\right)\right]^{2/(2+p)}. \tag{4.9}$$

For $p=2$ (harmonic oscillator), this formula reproduces the exact answer (with $\omega=\sqrt{3}$); for a linear potential ($p=1$) $E_{00}^v\simeq 3.87114$, which is 0.2% higher than the exact value (see the review in Ref. 5, which contains both variational estimates and the exact value for $p=1$). For $p=0.1$ Eq. (4.9) gives $E_0=1.88278$, which is 0.14% higher than the true vacuum state. Thus, $H^{(0)}$ is not a bad starting Hamiltonian for calculating the energy of the ground state.

Let us consider the first excited state of the Hamiltonian $H^{(0)}$ with the same symmetry as the ground state. This state is sometimes called $[56,0^+]'$. The wave function for $E=5\omega$ is

$$\Psi_{20}^{(0)}=\frac{1}{\sqrt{3\pi^3}}(\rho^2+\lambda^2-3)\exp\left[-\frac{\rho^2+\lambda^2}{2}\right]. \tag{4.10}$$

Repeating the above procedure, we find

$$E_{20}^v=5\left(\frac{2+p}{p}\right)\left[\frac{p(12+2p+p^2)}{40\sqrt{\pi}}\Gamma\left(\frac{3+p}{2}\right)\right]^{2/(2+p)}. \tag{4.11}$$

Again this formula reproduces the exact result $E_2=5\sqrt{3}$ for $p=2$; for $p=1$ the variational value $E_{20}^v\simeq 5.32593$ is 0.1% higher than the exact value $E_2=5.3207$ (see Ref. 5). For $p=0.1$, Eq. (4.11) gives a number that is 0.05% lower than the exact value cited in Refs. 1 and 11. Thus, it is reasonable to expect that the variational calculations (4.11) and (4.9) have errors of at most 0.5% for any p in the interval from 0 to 3, and can be used for estimates in the quark model.

In the same manner we can calculate higher and higher states, although the amount of effort expended grows rapidly with N. We have calculated, for example, the energy of the completely symmetric state with $N=4$, $L=0$ for the special case $p=1$. The results of our calculations can be found in Table V. We used the wave function

$$\Psi_{40}^{(0)}=\frac{1}{\sqrt{24\pi^3}}[(\rho^2+\lambda^2)^2-8(\rho^2+\lambda^2)+12]$$

$$\times\exp\left[-\frac{\rho^2+\lambda^2}{2}\right]. \tag{4.12}$$

The variational energy $E^v\simeq 6.6108$ differs from the exact value by 0.2%.[5]

TABLE V. Energy levels E_{NL} for a three-body system.

$L=0$									
	E^{v}_{00} (4.9)	E^{exact}_{00}	E^{asy}_{00} (4.21)	E^{v}_{20} (4.11)	E^{exact}_{20}	E^{asy}_{20} (4.21)	E^{v}_{40}	E^{exact}_{40}	E^{asy}_{40} (4.21)
$p=2$	5.1961	5.1961	5.1961	8.6603	8.6603	8.6603	–	12.1244	12.1244
$p=1$	3.8711	3.8631	3.8121	5.3259	5.3207	5.3587	6.6108	6.5953	6.7063
$p=0.1$	1.8828	1.8802	1.8587	1.9613	1.9589	1.9513		2.0143	2.0149

$L \neq 0$				
	E^{v}_{01} (4.15)	E^{exact}_{01}	E^{v}_{02} (4.18)	E^{exact}_{02}
$p=2$	6.9282	6.9282	8.6603	8.6603
$p=1$	4.7219	–	5.4670	–
$p=0.1$	1.9390	1.9362	1.9787	–

Note: The exact values are taken from Ref. 5. (A typographical error in Ref. 5 for E_{20} for $p=0.1$ has been corrected.)

Let us now consider the lowest state with $L=1$ and mixed permutation symmetry. The zeroth-approximation wave function has the form

$$\Psi^{\rho}_{11}=\frac{1}{\pi^{3/2}}(\rho_x+i\rho_y)\exp\left[-\frac{\rho^2+\lambda^2}{2}\right],$$

$$\Psi^{\lambda}_{11}=\frac{1}{\pi^{3/2}}(\lambda_x+i\lambda_y)\exp\left[-\frac{\rho^2+\lambda^2}{2}\right], \tag{4.13}$$

and the matrix element of the potential is

$$\langle\Psi^{\rho}_{11}|V|\Psi^{\rho}_{11}\rangle=\frac{3\cdot 2^{p/2}}{4}[\langle\Psi^{\rho}_{11}|\rho^p|\Psi^{\rho}_{11}\rangle+\langle\Psi^{\lambda}_{11}|\rho^p|\Psi^{\lambda}_{11}\rangle], \tag{4.14}$$

which leads to the following estimate for the energy of the state:

$$E^{v}_{1M}=4\left(\frac{2+p}{p}\right)\left[\frac{6(6+p)}{16\sqrt{\pi}}\Gamma\left(\frac{3+p}{2}\right)\right]^{2/(2+p)}. \tag{4.15}$$

We have also considered the lowest completely symmetric D state ($n=0, L=2$). The corresponding wavefunction of the harmonic oscillator is

$$\Psi^{s}_{22}=\frac{1}{2\pi^{3/2}}(\rho_+^2+\lambda_+^2)\exp-\left[\frac{\rho^2+\lambda^2}{2}\right], \tag{4.16}$$

the matrix element of ρ^p between these functions is equal to

$$\langle\rho^p\rangle_{22}=\frac{1}{\sqrt{\pi}}\left[\frac{1}{15}(30+8p+p^2)\right]\Gamma\left(\frac{3+p}{2}\right), \tag{4.17}$$

which leads to the following variational value of the energy for the symmetric D state:

$$E^{v}_{22}=5\left(\frac{2+p}{p}\right)\left[\frac{p}{100\sqrt{\pi}}(30+8p+p^2)\Gamma\left(\frac{3+p}{2}\right)\right]^{2/(2+p)}. \tag{4.18}$$

Let us now turn our attention to the asymptotic behavior (for large N) of the symmetric s-wave mode, using the three-particle harmonic oscillator. The corresponding classical motion is the motion of three particles in a plane when they always form an equilateral triangle. If we denote the position of the particles by $\mathbf{v}_i=\mathbf{A}_i\cos\omega t$, then the sum of the vectors $\mathbf{A}_i$ is zero, and the distance between any two particles is $|\mathbf{r}_{12}(t)|=\sqrt{3}\mathbf{A}\cos\omega t$. For the energy of the system $E=(N+3)\omega$ we can calculate A in terms of the energy E: $A=\sqrt{2(N+3)/3\omega}$, and thus

$$\langle r^{p}_{12}\rangle=(\sqrt{3}A)^p\frac{1}{\sqrt{\pi}}\frac{\Gamma((p+1)/2)}{\Gamma((p+2)/2)}. \tag{4.19}$$

As a result, the matrix element of the Hamiltonian is

$$\langle H\rangle=\tfrac{1}{2}(N+3)\omega+\tfrac{3}{2}\langle r^{p}_{12}\rangle, \tag{4.20}$$

which leads to the quasiclassical estimate

$$E^{asy}_{N0}=\frac{1}{2}\left(\frac{p+2}{p}\right)(N+3)^{2p/(2+p)}\times\left[\frac{3p}{\sqrt{\pi}2^{(2-p)/2}}\frac{\Gamma((1+p)/2)}{\Gamma((2+p)/2)}\right]^{2/(2+p)}, \tag{4.21}$$

where N is even. For $p=1$ this formula simplifies to

$$E^{asy}_{N0}(p=1)=3\left[\frac{3}{2\pi}(N+3)\right]^{2/3}=1.83266(N+3)^{2/3}. \tag{4.22}$$

Table V compares the asymptotic values (4.21) with the exact values for $N=0$, 2, 4 for various powers p. It can be seen that the accuracy of the asymptotic formulas is better than 2%, starting with $N=0$. Equation (4.21) indicates that the behavior of a three-body system in the symmetric state with $L=0$ for large N is analogous to the behavior of one particle in a linear potential (for $p=1$). The dependence $N^{2/3}$ can be obtained with the help of quasiclassical arguments in the formalism of hyperspherical functions; however, the following expansion term [3 in $(N+3)$] is specific for our calculation method with the help of the harmonic oscillator. In quasiclassical theory this constant is called the Maslov index. Thus, from Eq. (4.21) it follows that the Maslow index is equal to 3 in the three-body problem in three-dimensional space. There is one more way to convince oneself that the dependence on N suggested by Eq. (4.21) is valid. Thus, in

Ref. 11 the values of the energies for the first three symmetric states with $L=0$ were calculated for the potential with $p=0.1$ in five-dimensional space. Following our method with oscillators as a starting point, it is easy to see that in the quasiclassical region it is necessary to replace $N+3$ by $N+5$ in Eq. (4.21) in order to reproduce the variational estimates. This substitution gives the energy of the first three states with an accuracy of -1.9%, -1.3%, and -0.85%, respectively. In the normalization adopted in Ref. 11, $E_N=3.2394(N+5)^{0.095238}$, where $N=0, 2, 4,\ldots$ (In Ref. 10 the potential is given as Σr_{ij}^p whereas in Ref. 5 and in our work it is equal to $(1/2)\Sigma r_{ij}^p$).

Applications to the calculation of the baryon spectrum

It would be interesting to find a real-world application for the formulas we have obtained and compare the results with experimental data. Høgaasen and Richard[4] in 1983 considered one such possibility. They proposed to examine the ratio $(E_{1M}-E_{00})/(E_{20}-E_{00})$ (which we will denote as $R_1(p)$) and determine an empirical spectral index from the baryon spectrum. Using variational estimates (4.9), (4.10), and (4.15), we can find this ratio:

$$R_1(p)=\frac{E_{1M}^v-E_{00}^v}{E_{20}^v-E_{00}^v}=\frac{4\left(\dfrac{6+p}{8}\right)^{2/(2+p)}-3}{5\left(\dfrac{12+12p+p^2}{20}\right)^{2/(2+p)}-3} \qquad (4.23)$$

for $p>0$. Formula (4.23) reproduces the corresponding graph in Ref. 4 with an accuracy of 1% although the calculational methods are absolutely different. As was noted in Ref. 4, the baryon resonance data [with quantum numbers corresponding to Eq. (4.23)] do not correspond to any confinement potential. If we exclude the hyperfine interaction, then it follows from the data that $E_{00}\simeq 1135$ MeV, $E_{20}\simeq 1600$ MeV, and $E_{1M}\simeq 1610$ MeV (these numbers were obtained in Ref. 13). These values lead to the result $R_1(p)\simeq 1$, whereas in the region $0\leqslant p\leqslant 2$ the ratio $R_1(p)$ varies between 0.435 and 0.5. Thus, we run up against a serious difficulty. One possible way of resolving this problem begins by noting that it is unjustified to compare states with different permutation symmetry if the potential is not a simple function of r_{ij}, but also contains an interaction of the "string function" type. In order to investigate this possibility, we calculate the ratio $R_2(p)$, which includes only states completely symmetric under permutation:

$$R_2(p)=\frac{E_{22}^v-E_{20}^v}{E_{22}^v-E_{00}^v}, \qquad (4.24)$$

and which can be calculated by the variational method with the help of Eqs. (4.18), (4.9), and (4.10). As a result, we obtain

$$R_2(p)=\frac{\left[\dfrac{1}{50}(30+8p+p^2)\right]^{2/(2+p)}-\left[\dfrac{1}{20}(12+2p+p^2)\right]^{2/(2+p)}}{\left[\dfrac{1}{50}(30+8p+p^2)\right]^{2/(2+p)}-\dfrac{3}{5}}. \qquad (4.25)$$

The ratio $R_2(p)$ vanishes for $p=2$ (since $E_{22}=E_{20}$) and grows slowly with decreasing p up to $R_2(p)\simeq 0.19$ at $p\simeq 0$. The baryon resonance data give $E_{22}\simeq 1850$ MeV (Ref. 13), which leads to $R_2^{\mathrm{exp}}\simeq 0.35$. This experimental value is again quite far from being described in the potential model with a blocking potential in the range $0\leqslant p\leqslant 2$, and we, in essence, have the same problems for R_2 as were observed by Høgaasen and Richard[4] for R_1. The permutation symmetry bears no relation to these discrepancies from the experimental data, and we do not know of a solution to these two problems. We have tried, for example, to move the position of the s-wave excited state a little (by the width of the resonance, which is much wider than other resonances), in order to find the same p for $R_1(p)$ and $R_2(p)$. Such a general solution does not exist. It is possible that the P_{11} resonance is not a purely three-quark state, but contains, as Li proposed,[14] a significant admixture of the (qqq gluon) state. However, if this is true, then where is the $2s$ state?

5. CONCLUSION

We have shown how to extend the applicability of the variational method to the calculation of excited states for systems with a blocking potential. The errors in such calculations are small enough that this method can be used in practical problems, e.g., in baryon spectroscopy for lower excitations.

For high excitations this method gives the correct asymptotic form for the energy, which can be related to the classical variational principle for the mean Hamiltonian. The second advantage of the variational method is that it leads to states for which the virial theorem is satisfied. The main shortcoming of the method is that the states obtained using it are not orthogonal.

We have applied the variational method to the inverse problem in baryon spectroscopy, and confirmed and extended the negative result of Høgaasen and Richard.[4]

It is clear that the method, in principle, is also applicable to other problems, for example, the N-body problem with a blocking potential (i.e., with a discrete spectrum). It would also be very interesting to use it to examine the problem of quantum chaos.

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APPENDIX: VARIATIONAL PRINCIPLES IN CLASSICAL AND QUANTUM MECHANICS

In this Appendix we will discuss how variational principles in classical and quantum mechanics are related to our approximate variational calculations.

For simplicity, let us consider a system with one degree of freedom, executing periodic motion in the classical limit (i.e., for large quantum numbers n). Quantum averaging over the stationary state Ψ_n corresponds to classical averaging over time:

$$\langle H\rangle \equiv \langle \Psi_n|\hat{H}|\Psi_n\rangle \simeq \langle H\rangle_T \equiv \frac{1}{T}\int_0^T dt H(p(t),q(t)), \tag{A1}$$

where $(q(t),p(t))$ is the solution of the classical equations of motion for the system and T is the period. The classical analog of the statement that the system is found in the quantum state Ψ_n is that the classical solution $(q(t),p(t))$ satisfies the Sommerfeld–Wilson condition for the reduced action J:

$$J(T)=\int_0^T p(t)\dot{q}(t)dt=\oint p dq=\text{const.} \tag{A2}$$

According to the quantum variational principle, the eigenstates of the operator $\hat{H}$ are extrema of the functional $\langle H\rangle$ in Eqs. (A1):

$$\delta\langle H\rangle \equiv \delta\langle \Psi_n|\hat{H}|\Psi_n\rangle = 0, \tag{A3}$$

with the supplemental normalization condition

$$\langle \Psi_n|\Psi_n\rangle = 1,$$

where the subscript n indicates the Nth ($(n+1)$th) solution of Eq. (A3). The classical analog of this principle is the variational equation

$$\delta\langle H\rangle_T = 0 \tag{A4}$$

with the constraint

$$J=\oint p dq=\text{const.}$$

Here the extremum $\langle H\rangle_T$ is chosen from among the arbitrary periodic trial functions $p(t)$ and $q(t)$, generally speaking, with different period T, but the same value of the reduced action. (The variational procedure discussed in this paper pertains to a special class of trial functions—namely, solutions of the harmonic oscillator with frequency ω.)

The classical variational principle (A4) was postulated by Van Vleck[8] not long before the creation of quantum mechanics. We derive this principle classically from Hamilton's variational principle:

$$S(T)=\int_0^T dt(p\dot{q}-H(q,p)) \tag{A5}$$

for periodic functions $q(t)$:

$$q(0)=q(T). \tag{A6}$$

This boundary condition (A6) can be rewritten for the variation $\delta q(T)$:

$$\delta q(T+\delta T)=q(T)-q(T+\delta T),$$

or for small variations

$$\delta q(T)=-\dot{q}(T)\delta T. \tag{A7}$$

After this preliminary substitution it is easy to calculate the variation of $S(T)$ [Eq. (A5)]:

$$\delta S(T)=-H(T)\delta T+\int_0^T dt\left[\delta p\left(\dot{q}-\frac{\partial H}{\partial p}\right)-\delta q\left(\dot{p}+\frac{\partial H}{\partial q}\right)\right]. \tag{A8}$$

If we introduce the averaged action $\langle S\rangle$:

$$\langle S\rangle=\frac{1}{T}S(T)=\frac{1}{T}J-\langle H\rangle_T,$$

and consider only those variations δp, δq, and δT that conserve J, then we can rewrite Eq. (A8) in terms of the variation of the averaged energy $\langle H\rangle_T$:

$$\delta\langle H\rangle_T=\frac{\delta T}{T}[H(T)-\langle H\rangle_T]-\frac{1}{T}\int_0^T dt\left[\delta p\left(\dot{q}-\frac{\partial H}{\partial p}\right)-\delta q\left(\dot{p}+\frac{\partial H}{\partial q}\right)\right]. \tag{A9}$$

It is clear from Eq. (A9) that if $p(t)$ and $q(t)$ satisfy the equations of motion, then

$$\delta\langle H\rangle_T=0,$$

since $H(T)=\langle H\rangle_T$. On the other hand, if the left-hand side of Eq. (A9) vanishes for arbitrary variations δT, δp, δq, then it follows that the extrema satisfy Hamilton's equations and the energy conservation law $H(T)=\langle H\rangle_T$. In other words, the variational principle for the average energy is equivalent to Hamilton's principle for the class of trial functions with fixed J. From the classical point of view, it is most natural that the principle of Maupertuis arises from Hamilton's principle since the energy is conserved and can therefore be eliminated. As a result, we are left with the reduced action. From the quantum viewpoint, it is more natural to fix the reduced action; we are then left with a variational principle for the average energy.

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