Concavity of energy surfaces

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Abstract. The property of concavity in calculations of energy surfaces is developed and discussed, in reference to strict energy minimisation when collective coordinates are constrained. Such collective coordinates are actually subject to quantum fluctuations and these prevent, via tunnel effects, the probing of maxima and saddle points. A solution to the problem is developed. It allows to bypass the concavity syndrome and recover maxima and saddle points.

1. Introduction

For practical calculations in many-body physics, be they atomic, nuclear, molecular, or condensed matter, the concept of collective coordinates [1] has been of central importance. Its goal has been to generate models involving far fewer degrees of freedom than the true number, $3A$, as required for a proper, microscopic, description of a system of A particles. As is also often the case, the dynamics can be compressed into slow motions of a few collective degrees of freedom (B), while the other, faster, degrees of freedom are averaged out. Also, in the case of identical particles, such collective degrees of freedom may be represented as one-body operators: $B = \sum_{i=1}^{A} \beta(\mathbf{r}_i, \mathbf{p}_i, \sigma_i, \tau_i)$, where $\beta(\mathbf{r}_i, \mathbf{p}_i, \sigma_i,$ and τ_i refer to the individual particle i's position, momentum, spin, and, if necessary, isospin, respectively.

Once prescribed, such models lead to energy surfaces [2] of the system. Given the collective operator B with expectation value $b \equiv \langle B \rangle$, most collective models accept that there exists an energy function, $e(b)$, and an inertia parameter, $\mu(b)$, that drive the collective dynamics. Descriptions of such energy surfaces leads to terminology such as "saddles", "barriers", etc. [2, 3, 4].

Central to the prescription is the assumption that the energy function is a result of an energy *minimisation* under constraint. That is, while the system evolves through various values of b, it is accepted that the energy is tuned to achieve a (local) minimum. This aspect of finding the energy surface is central to many fields of physics. Consider a Hamiltonian, $H = \sum_i T_i + \sum_{i<j} V_{ij}$, where T and V denote the kinetic and potential energy operators. Given a trial set of density operators, $\mathcal{D}$, in many-body space and normalised by $\mathrm{Tr}\mathcal{D} = 1$, with Tr denoting the trace, the energy surface may be defined by

$$e(b) = \inf_{\mathcal{D} \Rightarrow b} \mathrm{Tr}\left\{H\mathcal{D}\right\}. \tag{1}$$

The constraint, $\mathcal{D} \Rightarrow b$, enforces $\mathrm{Tr}\left\{B\mathcal{D}\right\} = b$.

However, there are theories which do not use, *a priori*, energy minimisation for the "fast" degrees. Time-dependent Hartree-Fock (HF) trajectories [5], generalisations with pairing, adiabatic versions [6], often exhibit collective motions. Equations of motion [7] and/or a maximum decoupling [8] of "longitudinal" from "transverse" degrees of freedom, have also shown significant successes in the search for collective degrees. This has come at the cost, however, of imposing a one-body nature of both collective coordinates and momenta and accepting state-dependence of those operators. Such approaches define an energy surface once trajectories of wave functions in many-body spaces have been calculated. (They are not the subject of the present paper.) Herein, we focus on fixed operators constraining energy minimisation within a fixed basis for single-particle and many-body states.

To define properly am energy function $e(b)$ of the collective coordinate, one should first diagonalise B within the space defined by the many-body states. The resulting spectrum of B is assumed to be continuous, or at least have a high level density for the chose trial space. For each eigenvalue, b, one should then find the ground state energy eigenvalue $e(b)$, of the projection of H onto that eigensubspace labelled by b.

However, in practice, one settles for the diagonalisation of the constrained operator $\mathcal{H} = H - \lambda B$, where λ is a Lagrange multiplier, or, alternatively, for the minimisation of $\langle \mathcal{H} \rangle$. (This is not restricted to one constraint: one may add more constraints with suitable Lagrange multipliers defined.) B is assumed to have both lower and upper bounds, or, that the constrained Hamiltonian will always have a ground state. From that constrained Hamiltonian, one may obtain the free energy, $\varepsilon(\lambda) \equiv \langle \mathcal{H} \rangle$. The label b is no longer an eigenvalue but just an average value, as defined by the expectation value of B. A Legendre transform of $\langle \mathcal{H} \rangle$ then returns the energy surface $e(b)$, with b and λ forming a Legendre pair. Thus $d\varepsilon/d\lambda = -\mathrm{Tr}\left\{B\mathcal{D}\right\} = -b$ and $de/db = \lambda$. The problem lies when considering a constrained variation in a *quantum* system without additional precautions as: i) there is a link between strict minimisation and the curvature properties of $e(b)$; and ii) the usual interpretation of b as a well-defined coordinate for a collective model can be negated by non-negligible fluctuations (whatever the cause).

2. Theorem linking minimisation and concavity

Before proving the theorem, we must recall that, with Hartree-Fock (HF) and Hartree-Bogoliubov (HB) approximations, both concave and convex branches were obtained for $e(b)$ by replacing the constraint term, $-\lambda \langle B \rangle$, in $\langle \mathcal{H} \rangle$ by either $-\lambda' \langle B \rangle + \mu \langle B \rangle^2 /2$, [9], or $-C \left(\langle B \rangle - \mu\right)^2 /2$, [3, 4], with adjustable values of λ', C, and μ. However, both methods, while stabilizing the numerical procedure, amount to use an effective Lagrange multiplier, namely $\lambda_{\text{eff}} = \lambda - \langle B \rangle \mu$ and $\lambda_{\text{eff}} = C \left(\langle B \rangle - \mu\right)$, respectively. We shall, therefore, stick to the generic form, $H - \lambda B$, in the following.

Consider a solution branch $\mathcal{D}(\lambda)$, expanding up to second order, and assuming that the manifold of solutions is suitably analytic,

$$\mathcal{D}(\lambda + d\lambda) = \mathcal{D}(\lambda) + d\lambda(d\mathcal{D}/d\lambda) + (d\lambda^2/2)(d^2\mathcal{D}/d\lambda^2). \tag{2}$$

The stationarity and minimality of $\mathrm{Tr}\left\{\mathcal{H}\mathcal{D}\right\}$ with respect to any variation of $\mathcal{D}$, and in particular w.r.t. that variation, $\mathcal{D}(\lambda + d\lambda) - \mathcal{D}(\lambda)$, induce,

$$\begin{aligned} \mathrm{Tr}\left\{\mathcal{H} d\mathcal{D}/d\lambda\right\} &= 0, \\ \mathrm{Tr}\left\{\mathcal{H} d^2\mathcal{D}/d\lambda^2\right\} &\geq 0. \end{aligned} \tag{3}$$

The free energy ε is also stationary for $\mathcal{D}(\lambda + d\lambda)$, but the Hamiltonian is now, $\mathcal{H}(\lambda) - B d\lambda$, and the derivative of the state is, $d\mathcal{D}/d\lambda + d\lambda(d^2\mathcal{D}/d\lambda^2) + \mathcal{O}(d\lambda^2)$, hence,

$$\mathrm{Tr}\left\{(\mathcal{H} - B d\lambda)\left[d\mathcal{D}/d\lambda + d\lambda(d^2\mathcal{D}/d\lambda^2) + \mathcal{O}(d\lambda^2)\right]\right\} = 0. \tag{4}$$

The zeroth order of this, Eq. (4), is, $\mathrm{Tr}\left\{\mathcal{H}d\mathcal{D}/d\lambda\right\}$. It vanishes, because of the first of Eqs. (3). The first order, once divided by $d\lambda$, gives,

$$-\mathrm{Tr}\left\{Bd\mathcal{D}/d\lambda\right\} = -\mathrm{Tr}\left\{\mathcal{H}d^2\mathcal{D}/d\lambda^2\right\}. \tag{5}$$

The left-hand side of Eq. (5) is nothing but the the second derivative, $d^2\varepsilon/d\lambda^2$. The right-hand side is semi-negative-definite, because of the second of Eqs. (3). Hence, the plot of $\varepsilon(\lambda)$ is a convex curve and the plot of its Legendre transform, $e(b)$, is concave. (Other authors may have the opposite sign convention of the second derivative to define concavity versus convexity.) With our sign convention [10, 11], strict minimisation necessarily induces concavity, and any convex branch means that the "fast" degrees of freedom are not in a minimal energy.

It is important to note that this proof does not assume any specification of $\mathcal{D}(\lambda)$, whether it is constructed either from exact or approximate eigenstates of $\mathcal{H}$. Therefore strict minimisation can *only* return *concave* functions $e(b)$. Maxima are impossible. In the generalisation where several collective operators $B_1, \ldots, B_N$, are involved, concavity stills holds, so saddles are also excluded. Hence, only an absolute minimum is possible. (However, we shall show below how to overcome the paradox: by *keeping constant the fluctuations* of the collective coordinate(s), one can deviate from concavity, and more important, validate a constant quality of the representation provided by branches $\mathcal{D}(\lambda)$.)

Alternatively, let $\psi(\lambda)$ be the ground state of $\mathcal{H}$. (For the sake of simplicity, we assume that there is no degeneracy.) The corresponding eigenvalue, $\varepsilon(\lambda)$, is stationary with respect to variations of ψ, among which is the "online" variation, $d\lambda\,(d\psi/d\lambda)$, leading to the well-known first derivative, $d\varepsilon/d\lambda = -b \equiv -\langle\psi\,|B|\,\psi\rangle$. Consider the projectors $P = |\psi\rangle\langle\psi|$ and $Q = 1 - P$. Brillouin-Wigner theory yields the first derivative of ψ, *viz.*

$$\frac{d\,|\psi\rangle}{d\lambda} = -\frac{Q}{\varepsilon - Q\mathcal{H}Q}B\,|\psi\rangle. \tag{6}$$

This provides the second derivative of ε,

$$-\frac{db}{d\lambda} \equiv -\frac{d}{d\lambda}\langle\psi\,|B|\,\psi\rangle = 2\left\langle\psi\left|B\frac{Q}{\varepsilon - Q\mathcal{H}Q}B\right|\psi\right\rangle. \tag{7}$$

Since the operator $(\varepsilon - Q\mathcal{H}Q)$ is clearly negative-definite, the eigenvalue, ε, is a convex function of λ. It is trivial to prove that the same convexity holds for the ground state eigenvalue $\varepsilon(\lambda_1, \ldots, \lambda_N)$ if several constraints, $B_1, \ldots, B_N$, are used. If, moreover, a temperature T is introduced, the thermal state, $\mathcal{D} = \exp\left[-\mathcal{H}/T\right]/\mathrm{Tr}\exp\left[-\mathcal{H}/T\right]$, replaces the ground state projector, $|\psi(\lambda_1, \ldots, \lambda_N)\rangle\langle\psi(\lambda_1, \ldots, \lambda_N)|$, and the free energy, $\varepsilon(\lambda_1, \ldots, \lambda_N; T)$, also contains the entropy contribution, $-TS$, where $S = -\mathrm{Tr}\left\{\mathcal{D}\ln\mathcal{D}\right\}$. A proof of the convexity of the exact $\varepsilon(\lambda_1, \ldots, \lambda_N; T)$ is also easy [12].

At $T = 0$, the usual Legendre transform expresses the energy, $e \equiv \langle\psi\,|H|\,\psi\rangle$, in terms of the constraint value(s) rather than the Lagrange multiplier(s). For simplicity, consider one constraint only; the generalization to $N > 1$ is easy. Since $e \equiv \varepsilon + \lambda b$, then $de/db = \lambda$, a familiar result for conjugate variables. Furthermore, the second derivative, d^2e/db^2, reads, $d\lambda/db = 1/(db/d\lambda)$. From Eq. (7), the derivative, $db/d\lambda$, is positive-definite. Accordingly, e is a concave function of b. Now, if $T > 0$, the Legendre transform instead generates a reduced free energy, $\eta \equiv (e - TS)$, a concave function of the constraint value(s). An additional Legendre transform returns e alone, as a concave function of the constraint(s) and S.

Let b_- and b_+ be the lowest and highest eigenvalues of B. When λ runs from $-\infty$ to $+\infty$, then b spans the interval, $[b_-, b_+]$. There is no room for a junction with convex branches under technical modifications as used by [9, 3, 4]. For every exact diagonalization of $\mathcal{H}$, or

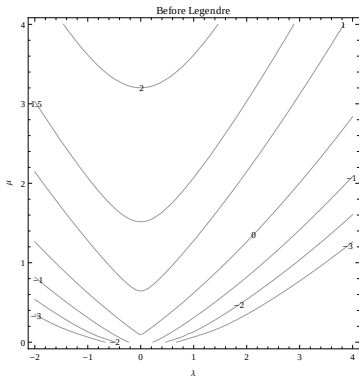

Figure 1. The convex contour plot of $\varepsilon(\lambda, \mu)$, for the model of Eq. (9).

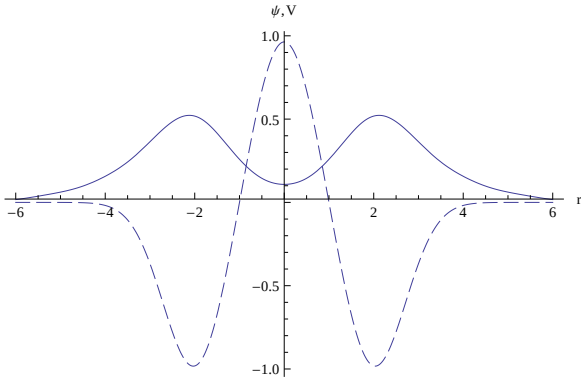

Figure 2. Ground state (solid line) when $\lambda = \mu = 0$, and potential (dashed line).

exact partition function, concavity sets a one-to-one mapping between b in this interval and λ. More generally, with exact calculations, there is a one-to-one mapping between the set of Lagrange multipliers, $\{\lambda_1, \ldots, \lambda_N\}$, and that of obtained values, $\{b_1, \ldots, b_N\}$, of the constraints. Concavity, *in the whole obtained domain of constraint values*, imposes a poor landscape: there is one valley only.

3. Results

With Q now denoting our generic constraint, we diagonlise $\mathcal{H} = H - \lambda Q$ accordingly, where the Lagrange multipler $\lambda \in (-\infty, \infty)$. This is equivalent to finding the roots of the equation $\mathcal{P}(\lambda, \varepsilon) \equiv \det(H - \lambda Q - \varepsilon) = 0$. We track of $\langle H \rangle$ and $\langle Q \rangle$, along the eigenstates of $\mathcal{H}$, *viz.*

$$\mathcal{Q}(\lambda, \varepsilon) \equiv \frac{\partial \mathcal{P}}{\partial \lambda} - \langle Q \rangle \frac{\partial \mathcal{P}}{\partial \varepsilon} = 0. \tag{8}$$

We replace ε in terms of $\langle H \rangle$, λ, and $\langle Q \rangle$, in $\mathcal{P}$ and $\mathcal{Q}$. By eliminating λ we obtain a resultant $\mathcal{R}(\langle H \rangle, \langle Q \rangle) = 0$. We plot $\langle H \rangle$ as a multi-valued function of $\langle Q \rangle$. (See Ref. [13] for details.)

Consider a model consisting of 11 (or 21) oscillators, where the Hamiltonian is

$$\begin{aligned} H &= \frac{P^2}{2} + V(r) \\ \mathcal{H} &= H - \lambda r + \mu r^2, \end{aligned} \tag{9}$$

which is a model with two constraints. Fig. 1, shows the (convex) contour plot of the lowest eigenvalue $\varepsilon(\lambda, \mu)$ of $\mathcal{H}$. Fig. 2 shows the ground state and potential energy of the model. If one allows for a fluctuation in r, denoted by Δr, as given in Fig. 3, one recovers the ground state energy landscape, Fig. 4, by subtracting the zero point energy. Figs. 5 and 6 show 3d plots of the energy as functions of constraints and of fluctuations, respectively. Concavity in the surface is clearly observed in Fig. 5, as is the shape of the potential in Fig. 6. Note that with increasing fluctuation the constraint is clearly lost.

4. Conclusions

There are problems in defining energy surfaces as a result of minimisations when constraints are subject to fluctuations. Controlling the effect of such fluctuations by second-order constraints is necessary to keep the quality of the energy across the landscape.

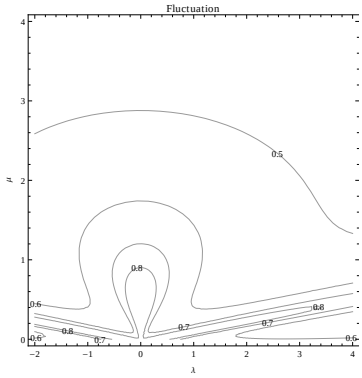

Figure 3. Contour plot of the fluctuation, Δr.

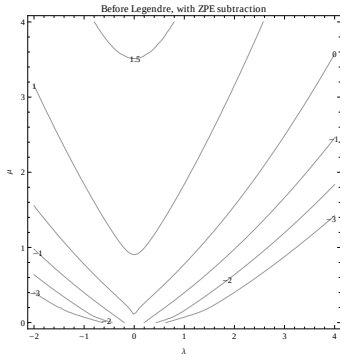

Figure 4. Contour of the ground state energy after subtraction of the zero point energy.

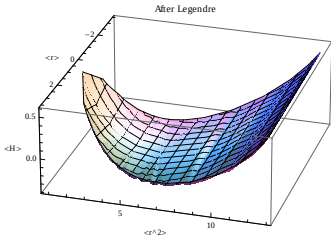

Figure 5. Constrained ground state as a function of $\langle r \rangle$ and $\langle r^2 \rangle$.

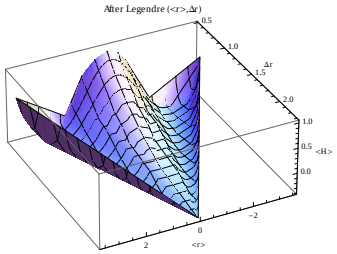

Figure 6. Same as Fig. 5, except as a function of $\langle r \rangle$ and Δr.

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