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Fluctuations of collective coordinates and convexity theorems for energy surfaces

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ABSTRACT

Constrained energy minimizations of a many-body Hamiltonian return energy landscapes $e(b)$ where $b \equiv \langle B \rangle$ represents the average value(s) of one (or several) collective operator(s), B, in an "optimized" trial state Φ_b, and $e \equiv \langle H \rangle$ is the average value of the Hamiltonian in this state Φ_b. It is natural to consider the uncertainty, Δe, given that Φ_b usually belongs to a restricted set of trial states. However, we demonstrate that the uncertainty, Δb, must also be considered, acknowledging corrections to theoretical models. We also find a link between fluctuations of collective coordinates and convexity properties of energy surfaces.

1. Introduction

Collective coordinates [1] have been of central importance in descriptions of structure and reactions in atomic, molecular, and nuclear physics. They generate models with far less degrees of freedom than the true number of coordinates, $3A$, as needed for a microscopic description of a system of A particles. Often, the system's dynamics can be compressed into slow motions of a few collective

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degrees of freedom B, while the other, faster degrees can be averaged out. Also, for identical particles, such collective degrees can be one-body operators, $B = \sum_{i=1}^{A} \beta(\mathbf{r}_i, \mathbf{p}_i, \sigma_i, \tau_i)$, where $\mathbf{r}_i$, $\mathbf{p}_i$, σ_i, τ_i refer to the position, momentum, spin, and if necessary isospin, respectively, of particle i. The summation over i provides for more inertia in B than in the individual degrees β_i.

The concept of energy surfaces [2] has been as important. Given a "coordinate-like" collective operator B and its expectation value $b \equiv \langle B \rangle$, most collective models use an energy function, $e(b)$, and also a b-dependent inertia parameter, that drive the collective dynamics. Keywords such as "saddles", "barriers", etc., flourish [2].

Simultaneously, it is often assumed that the function, $e(b)$, results from an energy *minimization* under constraint. Namely, while the system evolves through various values of b, it is believed to tune its energy to achieve a (local) minimum. This aspect of finding $e(b)$ is central to many fields of physics. To illustrate, consider a Hamiltonian, $H = \sum_i T_i + \sum_{i<j} V_{ij}$, where T and V denote the usual kinetic and interaction operators. Given a trial set of density operators, $\mathcal{D}$, in many-body space, normalized by $\mathrm{Tr}\mathcal{D} = 1$, the energy function $e(b)$ may be defined as,

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

where Tr is a trace in the many-body space for the A particles. The constraint, $\mathcal{D} \Rightarrow b$, enforces $\mathrm{Tr}\{B\mathcal{D}\} = b$.

There are theories which do not use, *a priori*, an axiom of energy minimization for the "fast" degrees of freedom. Time-dependent Hartree–Fock (HF) [3] trajectories, generalizations with pairing, adiabatic versions [4], often show collective motions. Equations of motion [5] and/or a maximum decoupling [6] of "longitudinal" from "transverse" degrees, have also shown significant successes in the search for collective degrees, at the cost, however, of imposing a one-body nature of both collective coordinates and momenta and accepting state-dependence of these operators. Such approaches define an energy surface once trajectories of wave functions have been calculated. But they are not the subject of the present analysis. Herein, we focus on fixed operators constraining strict energy minimizations within a fixed basis for single-particle and many-body states. The questions arise: are those constraints themselves subject to fluctuations, and what would be the effect of those fluctuations on the energy minimization?

These are not new questions. The issue of constrained Hartree–Fock calculations was addressed in Ref. [7], which considered constrained Hartree–Fock calculations, and corrections to the energy surface. The issue has also been considered more recently in relation to high-energy $(e, e'p)$ and $(p, 2p)$ reactions [8], where fluctuations in the position vectors of the target nucleons involved in those processes were considered as going beyond the mean-field approximation assumed for the structure of the target nucleus.

Ideally, to define mathematically a function $e(b)$ of the collective coordinate, one should first diagonalize B within the space provided by the many-body states available for calculations [9]. The resulting spectrum of B should be continuous, or at least have a high density for that chosen trial space. Then, for each eigenvalue b, one should find the lowest eigenvalue, $e(b)$, of the projection of H into that eigensubspace labeled by b.

In practice, however, one settles for a diagonalization of the constrained operator, $\mathcal{H} \equiv H - \lambda B$, where λ is a Lagrange multiplier, or at least for a minimization of $\langle \mathcal{H} \rangle$. Concomitantly, B is assumed to have both upper and lower bounds, or that the constrained Hamiltonian, $\mathcal{H}$, always has a ground state. This returns the "free energy", $\varepsilon(\lambda) \equiv \langle \mathcal{H} \rangle$. The label b is no longer an eigenvalue but just an average value, $b = \langle B \rangle$. A standard Legendre transform of $\varepsilon(\lambda)$ then yields the "energy surface", $e(b)$. This utilizes the properties $d\varepsilon/d\lambda = -\mathrm{Tr}\{B\mathcal{D}\} = -b$, and, $de/db = \lambda$. However we show in this work that constrained variation in a *quantum* system without additional precautions can raise at least two problems, namely: (i) the parameter b may no longer be considered as a well-defined coordinate for a collective model due to non-negligible fluctuations; we report cases where the uncertainties, Δb, can vitiate the meanings of both b and $e(b)$; and (ii) there is a link between *strict* minimization and the curvature properties of $e(b)$ when fluctuations are at work.

Our argument is based fundamentally on a few theorems, presented in Section 2, but also illustrated using a few explicit models, which may be solved analytically or numerically. Such