THE UNIQUE QUANTIZATION OF CLASSICAL HAMILTONIANS IN THE ADIABATIC TIME-DEPENDENT HF-THEORY

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Large amplitude collective phenomena are often described by means of a classical Hamiltonian $\mathcal{H}(q, p) = p^2/2\mathcal{M}(q) + \mathcal{V}(q)$, with $\mathcal{M}(q)$ being the collective mass and $\mathcal{V}(q)$ the collective potential. $\mathcal{H}$ is evaluated as expectation value of the microscopic Hamiltonian, $H(x_i, p_i)$, with a set of collectively deformed Slater determinants $\langle x_i | q, p \rangle$, where q is a collective coordinate and p its conjugate momentum. The basis $|q, p\rangle$ might be obtained, e.g., from the adiabatic TDHF[1,2]. It is the aim of this contribution to show that $\mathcal{H}$ can be quantized in a unique way, yielding the collective Hamiltonian

$$(1) \quad H_c = \frac{1}{4}\left(\hat{P}^2 \frac{1}{\mathcal{M}} + \beta \frac{1}{\mathcal{M}} \hat{P} + \frac{1}{\mathcal{M}} \hat{P}^2\right) + V(Q), \quad \hat{P} = -i\frac{\partial}{\partial Q} \; .$$

If there is a well developed collective channel, one can assume a grouping of the 3A coordinates x_i into a collective coordinate Q and intrinsic coordinates ξ_i. Then, H_c is that quantity which remains after averaging over the ξ_i. Hence all considerations can be restricted to a one-dimensional Q-space, representing, e.g., the collective basis $|q, p\rangle$ by a one coordinate wave function $\langle Q | q, p \rangle$. This "intrinsic" collective coordinate Q is to be identified with Q in H_c of eq.(1). Thus, the wave packet $\langle Q | q, p \rangle$ establishes the relation between $\mathcal{H}$ and H_c,

$$(2) \quad \mathcal{H}(q,p) = \langle q,p | \hat{H} | q,p \rangle = \int dQ \, \langle q,p | Q \rangle \, H_c \, \langle Q | q,p \rangle \; .$$

Since H_c is assumed to be of second order in p, $|q, p\rangle$ can be assumed to be of the form $|q, p\rangle = e^{ipQ}|q\rangle$. The remaining static wave packet $|q\rangle$ is determined by its Q-moments

$$(3) \quad \langle q,p | \hat{Q}^n | q,p \rangle = \int dQ \, \langle q,p | Q \rangle \, Q^n \, \langle Q | q,p \rangle$$

Now, H_c is to be defined such that it reproduces $\mathcal{H}$ in eq.(2) which implies an unfolding of the wave packet $\langle Q|q \rangle$ determined by eq.(3). This yields, up to second order in the moments $\langle Q^n \rangle$,

$$(4)\quad V = v - \frac{1}{4\beta} v'' - \frac{\beta}{4M}\,, \quad M = M\,, \quad \beta^{-1} = 2\langle Q^2 \rangle$$

(A generalization to higher orders is straightforward[3]). The potentials v and V differ essentially by the zero-point energy of the wave packet, whose consistent subtraction stabilises the process "classical limit and requantization". The particular p-ordering in eq.(1) is not compelling, but only convenient in the folding procedure. One can chose any other ordering, provided one changes the zero-point energy in V accordingly. The problem of p-ordering becomes irrelevant, if one considers kinetic and potential energy as a whole and carries through consistently the folding and defolding. The collective Schrödinger-equation with H_C will yield a solution $\Phi_C(Q)$. To be complete, one has to specify how to calculate matrix elements with Φ_C for a given operator. If we apply consistently the same defolding procedure as above, i.e. fixing the wave packet by eq.(3) and relating D_C with $\langle q, p | \hat{D} | q, p \rangle$ analogous to eq.(2), we obtain, e.g., for a static operator $\hat{D} = \hat{D}(x_i)$ the matrix element

$$(5)\quad \langle \alpha | \hat{D} | \beta \rangle = \int dQ\, \Phi_\alpha(Q)\, D_{C_i}\, \Phi_\beta(Q)\,,$$

$$D_{C_i} = \left(1 - \frac{1}{4\beta}\frac{\partial^2}{\partial q^2}\right) \langle q | \hat{D} | q \rangle\,.$$

References:

1. D.M. Brink, M.J. Giannoni, M. Veneroni, Nucl. Phys. A258 (1976) 237
2. K. Goeke, P.-G. Reinhard, preprint 1977
3. P.-G. Reinhard, Nucl. Phys. A252 (1975) 120