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# Semiclassical spectrum for a Hartree-type equation corresponding to a rest point of the Hamilton–Ehrenfest system

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**Abstract**

Following Ehrenfest's approach, the problem of quantum–classical correspondence can be treated in the class of trajectory-coherent functions that approximate a quantum-mechanical state as $\hbar \to 0$. This idea leads to a family of systems of ordinary differential equations, called Hamilton–Ehrenfest $M$-systems ($M = 0, 1, 2, \ldots$). As noted in the authors' previous works, every $M$-system is formally equivalent to the semiclassical approximation of order $M$ for the linear Schrödinger equation. In this paper a similar approach is undertaken for a nonlinear Hartree-type equation with a smooth integral kernel. It is demonstrated how quantum characteristics can be retrieved directly from the corresponding Hamilton–Ehrenfest systems, without solving the quantum equation: the semiclassical spectral series are obtained from the rest point solution. One of the key steps is derivation of a modified nonlinear superposition principle valid in the class of trajectory-coherent quantum states.

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## 1. Introduction

Semiclassical methods play a distinguished role among asymptotic approaches in linear mathematical physics. From the very beginning of quantum mechanics semiclassical approximation has been one of the main technical tools to address its two aspects: pragmatic and philosophical.

  

The pragmatic (computational) aspect relies on the presence of a *small* parameter $\hbar$ as a factor next to the derivatives. The pattern is demonstrated in the Schrödinger evolution equation

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \hat{\mathcal{H}}\Psi, \qquad \hat{\mathcal{H}} = \frac{\hat{\vec{p}}^{\,2}}{2m} + U(\vec{x}), \quad \hat{\vec{p}} = -\mathrm{i}\hbar\nabla_x, \quad \vec{x}\in\mathbb{R}^n, \tag{1.1}$$

corresponding to the classical Hamilton function

$$\mathcal{H}(\vec{p},\vec{x},t) = \frac{\vec{p}^{\,2}}{2m} + U(\vec{x}). \tag{1.2}$$

While Planck's $\hbar$ is a dimensional constant, there exists a large class of quantum-mechanical problems where a small dimensionless parameter, proportional to $\hbar$, is present. Accordingly, there is a mathematical problem to construct an approximate (with respect to that parameter) solution of the quantum-mechanical equation. Such an approximate solution is traditionally termed *the semiclassical asymptotics as* $\hbar\to 0$.

The philosophical aspect is related to the correspondence principle, one of the cornerstones of quantum mechanics. Despite the fact that quantum mechanics in its axiomatic formalization is a self-consistent theory and does not appeal to the classical mechanics, the correspondence principle requires the classical equations of motion to emerge from the quantum theory in the limit $\hbar\to 0$.

Obviously, there is no universal (i.e. physical problem independent) way to obtain arbitrary classical values from quantum-mechanical values. In each particular case, it is necessary to specify in what sense a quantum characteristic becomes classical as $\hbar\to 0$. The problem of deriving classical equations of motion from those of quantum mechanics in the limit $\hbar\to 0$ is one of the principal questions of the quantum–classical correspondence.

Historically, there are a number of approaches to the problem. One of them is due to Born [1], in which a quantum system is approximately described by the classical statistical ensemble expressed via a semiclassical wavefunction. A justification of this approach is based on the construction of a semiclassical solution to the quantum equation. The time-global version of such a construction is known as the Maslov canonical operator [2, 3]. In this approach the correspondence principle reveals itself in the fact that the principal term of the asymptotic expansion of the quantum density matrix is a solution of the classical Liouville equation.

Another approach, suggested by Ehrenfest [4], is based on the idea that Newtonian equations of motion can be obtained in the limit $\hbar\to 0$ from equations for mean values of the corresponding quantum-mechanical observables. More generally, any ordinary differential equations (ODE) obtained in the same manner from equations of quantum mechanics can be called classical. The correspondence between a quantum observable and its classical counterpart (assuming that such exists) is understood as follows: the quantum mean value $\langle\hat{A}\rangle_\Psi$ of the observable $\hat{A} = A(\hat{z},\hbar)$ calculated with respect to some special non-stationary states $\Psi(t;\hbar)$ must yield in the limit $\hbar\to 0$ the corresponding classical observable $A$ evaluated on a certain classical trajectory $z(t)$ in the phase space

$$\lim_{\hbar\to 0}\langle\hat{A}\rangle_\Psi = A(z(t),0). \tag{1.3}$$

Here and later by $z$ we denote the $2n$-vector $(\vec{p},\vec{x})$. For the Schrödinger equation (1.1) the Ehrenfest approach relies on states $\Psi(\vec{x},t;\hbar)$ that are *localized on the classical trajectory* in the following sense: the mean values

$$\begin{aligned}\bar{x}_k(t,\hbar) &\equiv \langle\hat{x}_k\rangle_\Psi = \int_{\mathbb{R}^n} x_k|\Psi|^2\,\mathrm{d}\vec{x},\\ \bar{p}_k(t,\hbar) &\equiv \langle\hat{p}_k\rangle_\Psi = \int_{\mathbb{R}^n}\Psi^*\hat{p}_k\Psi\,\mathrm{d}\vec{x}, \qquad k=1,\dots,n,\end{aligned} \tag{1.4}$$

of the operators of coordinates $\hat{\vec{x}} = (x_1, \dots, x_n)$ and momenta $\hat{\vec{p}} = -i\hbar\nabla$ calculated with respect to such states $\Psi(x, t; \hbar)$ in the limit $\hbar \to 0$

$$X_k(t) = \lim_{h\to 0} \bar{x}_k(t, \hbar), \qquad P_k(t) = \lim_{h\to 0} \bar{p}_k(t, \hbar), \qquad k = 1, \dots, n, \quad (1.5)$$

obey the classical Hamiltonian system

$$m\ddot{\vec{X}} = \vec{P}, \qquad \dot{\vec{P}} = -\nabla_x U(\vec{X}). \quad (1.6)$$

A function $\Psi$ for which the limits (1.5) exist was called in [5, 6] a *trajectory-coherent state*.

The technical implementation of the Ehrenfest approach is based on the construction of either exact or approximate trajectory-coherent solutions of the Schrödinger equation. Exact trajectory-coherent solutions are available only for special Hamiltonians, such as (1.1) with quadratic potential. Examples are well-known coherent and squeezed coherent states [7, 8]. An approximate ($\hbar \to 0$) trajectory-coherent solution, called a *semiclassically concentrated state* can be constructed in a much wider class of problems, employing the ideas of the complex WKB–Maslov method [9, 10] (see also [11–14]). The correspondence principle is manifested in this construction: a trajectory-coherent state is an approximate ($\hbar \to 0$) solution of (1.1) (i.e. it is a semiclassically concentrated state) if and only if the trajectory (1.5) satisfies the classical equation (1.6). The semiclassically concentrated states were first found for particles moving in a potential field [15], and later in an arbitrary electromagnetic field [5, 6]. Detailed bibliography can be found in the reviews [14, 16].

It was found that semiclassically concentrated states exist for linear equations of quantum mechanics describing a charged particle with spin or isospin in an external field. In [17–21] the semiclassically concentrated states were constructed for the Klein–Gordon and Dirac–Pauli equations in an arbitrary electromagnetic field as well as for the Schrödinger and Dirac equations in an arbitrary non-Abelian field with gauge group $SU(2)$.

The existence of the semiclassically concentrated states is essential for the approach employed in this paper, which consists of the following. Consider an observable $\hat{A} = A(\hat{z})$ whose classical analogue is $A(z)$. Its mean value in a semiclassically concentrated state can be expressed to any accuracy $O(\hbar^{(M+1)/2})$ via a solution $\{z(t), \Delta^2(t), \dots, \Delta^M(t)\}$ of a finite system of ODEs,

$$\langle \hat{A} \rangle_\Psi = A(z(t)) + \sum_{k=2}^{M} A_k(z(t)) \cdot \Delta^k(t) + O(\hbar^{(M+1)/2}), \qquad \Delta^k(t) = O(\hbar^{k/2}), \quad (1.7)$$

where tensors $A_k(z)$ comprise all partial derivatives of $A$ of order $k$ at the point $z$, and tensors $\Delta^k$ comprise all moments of order $k$ (see (1.9)).

The dimension of the ODE system is determined by the order of accuracy $M$. For instance, if $M = 0$ or 1 (it appears that $\Delta^1 = 0$ by construction), we obtain

$$\langle \hat{A} \rangle_\Psi = A(z(t)) + O(\hbar),$$

where $z(t)$ is subject to classical-mechanics equations, in accordance with Ehrenfest's original idea (1.3). In our approach, by classical equations (of order $M \geqslant 0$) corresponding to a quantum equation we mean that finite system of ODEs whose solution provides accuracy $O(\hbar^{(M+1)/2})$ in (1.7), and we call it the *Hamilton–Ehrenfest M-system*.

The Hamilton–Ehrenfest systems of finite order are truncations of an infinite ODE system, which describes evolution of the mean values for a basic infinite set of observables. For the Schrödinger equation (1.1) the basic set consists of $\hat{\vec{x}}$, $\hat{\vec{p}}$ and a special basis of the universal enveloping of the Heisenberg–Weyl algebra with generators $\hat{I}$, $\Delta\hat{x}_k = \hat{x}_k - \bar{x}_k(t)$, $\Delta\hat{p}_k = \hat{p}_k - \bar{p}_k$, $1 \leqslant k \leqslant n$, where $\hat{I}$ is the identity operator and $\bar{x}_k$, $\bar{p}_k$ are defined in (1.4).

The truncations leading to $M$-systems are made due to the estimates for $\Delta^k$ in (1.7), which allow us to disregard within given accuracy $O(\hbar^{(M+1)/2})$ all variables $\Delta^k$ for $k > M$ when the means are calculated with respect to semiclassically-concentrated states. The $M = 0$ truncation is simply Newton's system (1.6); similarly, the Hamilton–Ehrenfest 0-system for the Klein–Gordon equation is the Lorentz equation.

The infinite ODE system for (1.1) was derived in [22–24] and it was called the Hamilton–Ehrenfest system in [16]. The name reflects a non-trivial fact that the infinite system can be written in the Hamiltonian form with respect to a degenerate nonlinear Dirac bracket [25]. A system with a similar algebraic structure was also derived for the (matrix) Pauli equation [26]. A Hamiltonian structure with a degenerate Poisson bracket is also known for the $M = 2$ truncation [25, 27, 28]. The truncated systems were independently introduced in [29] and used to study quantum problems with underlying classically chaotic dynamics.

In a number of examples this approach was shown to agree with known 'classical' equations of motion even in the cases where no corresponding classical observables existed. For the Dirac–Pauli equation in an external field the Hamilton–Ehrenfest 0-system is a pair of classical equations which are the Lorentz equation and the Bargmann–Michel–Telegdi [30] equation in which the field is calculated on the trajectories of the Lorentz equation. The order $M = 2$ truncation obtained in [21] is a Frenkel-type [31] ODE for spin motion. For the Schrödinger and Dirac equations in external fields with gauge group $SU(2)$ the Hamilton–Ehrenfest 2-system [18, 20] yields the Wong equation [32] for a non-Abelian particle with isospin $1/2$. More examples of derivations of known 'classical' equations from the Dirac equation with external fields and the Proca equation are given in [33–35].

The Hamilton–Ehrenfest $M$-system is semiclassically equivalent with accuracy $O(\hbar^{(M+1)/2})$ to the Schrödinger equation in the class of trajectory-coherent states in the sense that it allows us to calculate the mean value of an observable directly from the solutions of the system. An explicit formula for the state is not required. It was also observed that under certain conditions one can obtain asymptotics for pure quantum characteristics, such as energy spectrum series, from stationary or periodic solutions of the Hamilton–Ehrenfest 2-system.

The goal of this paper is to generalize the approach for the case of a nonlinear Hartree-type equation. In particular, we can consider the following equation of self-consistent field (in fact, we deal with more general equations (2.1), (2.2))

$$\begin{aligned} &\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \widehat{\mathcal{H}}_\varkappa(\Psi)\Psi, \\ &\widehat{\mathcal{H}}_\varkappa(\Psi) = -\frac{\hbar^2}{2m}\nabla_x^2 + U(\vec{x}) + \varkappa\int_{\mathbb{R}^n} V(\vec{x},\vec{y})|\Psi(\vec{y},t)|^2\,\mathrm{d}\vec{y}, \qquad \vec{x}\in\mathbb{R}^n, \end{aligned} \tag{1.8}$$

where $U(\vec{x})$ and $V(\vec{x},\vec{y})$ are given smooth potentials of the external electromagnetic field and the self-consistent field respectively, and $\varkappa$ is a constant.

There are at least two reasons why the problem of quantum–classical correspondence was not considered in the spirit of Ehrenfest's approach, neither for a nonlinear self-consistent field (1.8), nor for more general Hartree-type equations.

First, the operator $\widehat{\mathcal{H}}_\varkappa(\Psi)$ does not have a natural classical analogue in the traditional sense, thus it is not *a priori* obvious which dynamical $\Psi$-independent system is an appropriate candidate for the 'classical' system in the limit $\hbar \to 0$.

Second, it is not clear whether the nonlinear quantum equation has either exact or approximate (as $\hbar \to 0$) solutions that are trajectory-coherent in the sense of (1.5).

In the framework of our approach, a solution of the correspondence problem includes three stages.

(1) First, for an arbitrary one-parameter family of phase-space trajectories $Z(t,\hbar) = (\vec{P}(t,\hbar), \vec{X}(t,\hbar))$, $t \in \mathbb{R}$, we introduce a class $\mathcal{P}^t_\hbar(Z(t,\hbar))$ of *trajectory-coherent* (also known as *trajectory-concentrated*) *functions*. Exact construction is given in section 3.

Let $\alpha, \beta \in \mathbb{Z}^n_+$ be multi-indices, $|\alpha| = \sum_{k=1}^n \alpha_k$, and $\vec{X}^\alpha = \prod_{j=1}^n X_j^{\alpha_j}$. Let $\widehat{\Delta}_{\alpha\beta}$ be an operator with Weyl symbol $\Delta_{\alpha\beta}(\vec{p},\vec{x}) = (\vec{x} - \vec{X}(t))^\alpha (\vec{p} - \vec{P}(t))^\beta$. The following property is essential for further steps: the centred moments

$$\Delta_{\alpha\beta}(t,\hbar) = \langle \widehat{\Delta}_{\alpha\beta} \rangle_\Psi, \tag{1.9}$$

calculated with respect to functions from class $\mathcal{P}^t_\hbar(Z(t,\hbar))$ satisfy the estimate

$$\Delta_{\alpha\beta} = O(\hbar^{(|\alpha|+|\beta|)/2}), \qquad \hbar \to 0.$$

Consequently, $k$th order moments (i.e. those with $|\alpha| + |\beta| = k$) are $O(\hbar^{k/2})$.

(2) Next, we assume that equation (1.8) has either an exact or approximate (with accuracy $O(\hbar^{(M+1)/2})$, $M \geqslant 0$) solution $\Psi$ in the class of trajectory-coherent functions. Using an approach similar to the linear case, we derive an infinite Hamilton–Ehrenfest system for the nonlinear equation (1.8) and its finite $M$-truncations for $\{(\vec{P}(t,\hbar), \vec{X}(t,\hbar)), \Delta_{\alpha\beta}(t,\hbar), |\alpha| + |\beta| \leqslant M\}$. Details are provided in section 4. In particular, the principal ($M = 0$) Hamilton–Ehrenfest system for the nonlinear equation of self-consistent field has the form

$$m\ddot{\vec{X}} = \vec{P}, \qquad \dot{\vec{P}} = -\nabla_x U(\vec{X}) - \varkappa \nabla_x V(\vec{x},\vec{y})|_{\vec{y}=\vec{x}=\vec{X}}. \tag{1.10}$$

Note that when $\varkappa = 0$, this system turns to (1.6). Similarly to the latter, the system (1.10) describes with accuracy $\hbar^{1/2}$ the trajectory where the trajectory-coherent solution $\Psi \in \mathcal{P}^t_\hbar$ is localized.

(3) Given a semiclassically-concentrated solution of equation (1.8) with accuracy $O(\hbar^{(M+1)/2})$, one can obtain a corresponding solution to the Hamilton–Ehrenfest system of order $M$ by evaluating mean values of operators $\hat{\vec{x}}$, $\hat{\vec{p}}$, $\widehat{\Delta}_{\alpha\beta}$ with respect to that solution. Our goal is to show that it works the other way around as well: quantum characteristics can be found with accuracy $O(\hbar^{(M+1)/2})$ from a solution of the Hamilton–Ehrenfest $M$-system.

In section 5 we study the Hamilton–Ehrenfest 2-system for the Hartree-type equation and in particular its stationary solution. Based on this calculation, in section 6 we construct the asymptotical energy spectrum for the Hartree-type equation. Examples in section 7 illustrate general results.

The key point of the whole approach is to obtain quantum characteristics without explicitly solving the quantum-mechanical equation. An explicit formula for the solutions is not required anywhere in the derivation. A basic assumption of the paper is the existence of a semiclassically concentrated solution of the Hartree-type equation in a class $\mathcal{P}^t_\hbar$. This assumption can be justified by explicit construction of formal asymptotic solutions using finite-dimensional Hamilton–Ehrenfest systems [36–40].

## 2. Hartree-type equation

By the Hartree-type equation we mean the following equation:

$$\{-\mathrm{i}\hbar\partial_t + \hat{\mathcal{H}}_\varkappa(\Psi)\}\Psi = 0, \qquad \hat{\mathcal{H}}_\varkappa(\Psi) = \hat{\mathcal{H}} + \varkappa\hat{V}(\Psi), \qquad \Psi \in L_2\big(\mathbb{R}^n_x\big). \tag{2.1}$$

Here

$$\hat{\mathcal{H}} = \mathcal{H}(\hat{z}), \qquad \hat{V}(\Psi) = \int_{\mathbb{R}^n} \mathrm{d}\vec{y}\, \Psi^*(\vec{y},t) V(\hat{z},\hat{w}) \Psi(\vec{y},t), \tag{2.2}$$

where the pseudo-differential operators $\mathcal{H}(\hat{z})$ and $V(\hat{z},\hat{w})$ with symbols $\mathcal{H}(z)$ and $V(z,w)$ respectively are functions of non-commuting sets of operators

$$\hat{z} = (-\mathrm{i}\hbar\nabla_x, \vec{x}), \qquad \hat{w} = (-\mathrm{i}\hbar\nabla_y, \vec{y}), \qquad \vec{x}, \vec{y} \in \mathbb{R}^n,$$

Function $\Psi^*$ is the complex conjugate to $\Psi$, $\varkappa$ is a real parameter, $\hbar > 0$ is a small parameter. The operators $\hat{z}$ and $\hat{w}$ satisfy the canonical commutation relations

$$[\hat{z}_k, \hat{z}_j] = [\hat{w}_k, \hat{w}_j] = \mathrm{i}\hbar J_{kj}, \tag{2.3}$$

$$[\hat{z}_k, \hat{w}_j] = 0, \qquad k, j = 1, \ldots, 2n, \tag{2.4}$$

where $J = \|J_{kj}\|_{2n\times 2n}$ is the standard symplectic matrix

$$J = \begin{pmatrix} 0 & -\mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}_{2n\times 2n},$$

and $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ denotes the commutator of $\hat{A}$ and $\hat{B}$.

In this paper all functions of non-commuting operators are Weyl-ordered [41, 42]. The action of the operator $\hat{\mathcal{H}}$ in this case can be written as

$$\hat{\mathcal{H}}\Psi(\vec{x}, t, \hbar) = \frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{2n}} \mathrm{d}\vec{y}\,\mathrm{d}\vec{p}\,\exp\left(\frac{\mathrm{i}}{\hbar}\langle\vec{x}-\vec{y}, \vec{p}\rangle\right)\mathcal{H}\left(\vec{p}, \frac{\vec{x}+\vec{y}}{2}\right)\Psi(\vec{y}, t, \hbar), \tag{2.5}$$

where $\mathcal{H}(z) = \mathcal{H}(\vec{p}, \vec{x})$ is the Weyl symbol of the operator $\hat{\mathcal{H}}$, and $\langle\vec{x}, \vec{p}\rangle = \sum_{k=1}^{n} x_k p_k$.

**Remark .** In the particular case when the Weyl symbols of operators $\mathcal{H}(\hat{z})$ and $V(\hat{z}, \hat{w})$ in (2.2) have the form

$$\mathcal{H}(z) = \frac{\vec{p}^2}{2m} + U(\vec{x}), \qquad V(z, w) = V(\vec{x}, \vec{y})$$

equation (2.1) yields the equation of self-consistent field in the form (1.8). This differential equation with integral nonlinearity plays a fundamental role in quantum theory and nonlinear optics [45, 46] and in the Bose–Einstein condensate theory [47]. In the latter the solution $\Psi$ represents the wavefunction of the condensate, while the non-local potential $V(\vec{x}, \vec{y})$ describes the interaction of condensate's particles with an external field.

In this paper we deal with asymptotic solutions of the equation (2.1) localized in the usual mathematical sense rather than in the sense of (1.5): namely, functions or formal series $\Psi(\vec{x}, t, \hbar)$ must belong to the Schwartz space with respect to the variables $\vec{x} \in \mathbb{R}^n$. We require the Weyl symbols $\mathcal{H}(z)$ and $V(z, w)$ of the operators $\hat{\mathcal{H}}$ and $V(\hat{z}, \hat{w})$ in (2.2) to belong to one of the $T^m_+$ classes [3, p. 13]: they must be smooth functions of at most polynomial growth with all derivatives, such that the following conditions hold.

**Assumption 1.** *The functions $\mathcal{H}(z)$ and $V(z, w)$ are infinitely differentiable for all $z \in \mathbb{R}^{2n}$ and $w \in \mathbb{R}^{2n}$, and for any multi-indices $\alpha, \mu \in \mathbb{Z}^{2n}_+$ there exist constants $C_\alpha$, $C_{\alpha\mu}$ and $m \geqslant 0$ such that*

$$\left|\frac{\partial^{|\alpha|}\mathcal{H}(z)}{\partial z^\alpha}\right| \leqslant C_\alpha(1+|z|)^m, \qquad \left|\frac{\partial^{|\alpha+\mu|}V(z, w)}{\partial z^\alpha \partial w^\mu}\right| \leqslant C_{\alpha\mu}(1+|z|)^m(1+|w|)^m.$$

The notation here is as follows:

$$\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_{2n}), \qquad \alpha_j \geqslant 0, \qquad |\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_{2n},$$
$$z^\alpha = z_1^{\alpha_1} z_2^{\alpha_2} \cdots z_{2n}^{\alpha_{2n}}, \qquad \frac{\partial^{|\alpha|}V(z)}{\partial z^\alpha} = \frac{\partial^{|\alpha|}V(z)}{\partial z_1^{\alpha_1}\partial z_2^{\alpha_2}\cdots\partial z_{2n}^{\alpha_{2n}}}. \tag{2.6}$$

Note that for our method it is essential to have smooth symbols $\mathcal{H}(z)$ and $V(z, w)$. Asymptotics for Hartee-type equations with singularities are a subject of a number of publications (see e.g. [43] and references therein).

Now we introduce a vector space in which asymptotic solutions to equation (2.1) will be sought.

## 3. Class of trajectory-coherent functions

We will construct asymptotic solutions of equation (2.1) with the following features: they have a form of wave packets and singularly depends on the small parameter $\hbar \to 0$.

Such a solution relies on a phase-space trajectory $Z(t,\hbar) = (\vec{P}(t,\hbar), \vec{X}(t,\hbar))$ and is trajectory-coherent in the sense of (1.4), (1.5). We denote the class of trajectory-coherent (trajectory-concentrated) functions by $\mathcal{P}^t_\hbar(Z(t,\hbar))$ and define it as

$$\mathcal{P}^t_\hbar = \mathcal{P}^t_\hbar(Z(t,\hbar)) = \left\{\Phi : \Phi(\vec{x},t,\hbar) = \varphi\left(\frac{\Delta\vec{x}}{\sqrt{\hbar}}, t, \hbar^{1/2}\right)\exp\left[\frac{\mathrm{i}}{\hbar}(S(t,\hbar) + \langle\vec{P}(t,\hbar), \Delta\vec{x}\rangle)\right]\right\}, \tag{3.1}$$

where function $\varphi(\vec{\xi}, t, \hbar^{1/2})$ belongs to the Schwartz space $\mathcal{S}$ with respect to variables $\vec{\xi} \in \mathbb{R}^n$, is a smooth function of $t$ and regularly depends on $\hbar^{1/2}$ as $\hbar \to 0$ (the term *function* is used throughout in the following, although $\varphi(\vec{\xi}, t, \hbar^{1/2})$ may in fact be a *formal series* in powers of $\hbar^{1/2}$). Here $\Delta\vec{x} = \vec{x} - \vec{X}(t,\hbar)$. The real function $S(t,\hbar)$ and the $2n$ component vector-function $Z(t,\hbar)$ also regularly depend on $\hbar$ as $\hbar \to 0$. When an asymptotic solution of equation (2.1) is being constructed, these functions, as well as the amplitude $\varphi(\vec{\xi}, t, \hbar^{1/2})$ are to be determined. We stress that the sub- and superscripts $\hbar, t$ in the notation of the class $\mathcal{P}^t_\hbar(Z(t,\hbar))$ just symbolize the dependence of the elements of this space on the corresponding parameters, as opposed to the functional parameter $Z(t,\hbar)$, which distinguishes different *classes* of the same nature. Simply put, the trajectory $Z(t,\hbar)$ is fixed but the values $t$ and $\hbar$ are not. To be definite, we assume $\hbar \in (0, 1]$. A short notation $\mathcal{P}^t_\hbar$ for $\mathcal{P}^t_\hbar(Z(t,\hbar))$ will be used when it does not lead to a confusion.

The class $\mathcal{P}^t_\hbar(Z(t,\hbar))$ is a vector space in the *algebraic* sense. Its elements are formal series in powers of $\hbar^{1/2}$ whose coefficients are smooth functions of the arguments $t$, $x$ and the operations of addition and scalar multiplication are performed term-wise. The formal series may not necessarily have a definite numerical value for the given values of $x$, $t$ and $\hbar$; however we want to use the familiar symbols of modulus ($|\cdot|$) and norm ($\|\cdot\|$), as well as inner products etc. All these objects will be understood as formal series in powers of $\hbar^{1/2}$ defined term-wise. The norm $\|\cdot\|$ always means the $L_2$-norm calculated with respect to $x$ variables for each fixed $t$. In most cases only the order of magnitude in $\hbar$ will be of importance and it will not depend on $t$. In such cases we write, for example, $\|\Phi(t)\|^2 = \|\Phi\|^2$, omitting the argument $t$.

It appears [37] that the functions $Z(t,\hbar)$ and $S(t,\hbar)$ are uniquely determined by the Hamilton–Ehrenfest system corresponding to the Hamiltonian of equation (2.1). In the linear case ($\varkappa = 0$) the vector function $Z(t,0)$ and the scalar function $S(t,0)$, defined by the Hamiltonian function $\mathcal{H}(\vec{p},\vec{x})$, are the classical-mechanics phase-space trajectory and the classical action respectively. As a sample amplitude, a Gaussian dynamical coherent state for quadratic Hamiltonians can be given:

$$\varphi(\vec{\xi}, t) = \exp\left[\frac{\mathrm{i}}{2}\langle\vec{\xi}, Q(t)\vec{\xi}\rangle\right] f(t),$$

where $Q(t)$ is a complex symmetric matrix with a positive imaginary part, and the time-dependent factor $f(t)$ is given by

$$f(t) = \sqrt[4]{\det \operatorname{Im} Q(t)}\exp\left[-\frac{\mathrm{i}}{2}\int_0^t \operatorname{Sp}\operatorname{Re} Q(\tau)\,\mathrm{d}\tau\right]$$

(see [16] for details).

Let us list important properties of functions from the class $\mathcal{P}^t_\hbar$. Proofs can be found in [16]; we sketch some of them in appendix B.

(1) Let $\Phi \in \mathcal{P}^t_\hbar(Z(t,\hbar))$. Let $\alpha \in \mathbb{Z}^{2n}_+$ denote a multi-index with $2n$ non-negative integer components $\alpha_j \in \mathbb{Z}_+$, $j = 1, \ldots, 2n$. Introduce operator $\{\Delta\hat{z}\}^\alpha$ with Weyl symbol $(\Delta z)^\alpha = (\Delta z_1)^{\alpha_1} \cdot \ldots \cdot (\Delta z_{2n})^{\alpha_{2n}}$, and

$$\Delta z = z - Z(t,\hbar) = (\Delta\vec{p}, \Delta\vec{x}), \qquad \Delta\vec{p} = \vec{p} - \vec{P}(t,\hbar), \qquad \Delta\vec{x} = \vec{x} - \vec{X}(t,\hbar).$$

Then the following asymptotic estimations for moments $\Delta_\alpha(t,\hbar)$ of order $|\alpha| = \sum_{j=1}^{2n} \alpha_j$ hold,

$$\Delta_\alpha(t,\hbar) = \frac{\langle\Phi|\{\Delta\hat{z}\}^\alpha|\Phi\rangle}{\|\Phi\|^2} = O(\hbar^{|\alpha|/2}), \qquad \hbar \to 0. \tag{3.2}$$

Here $\langle\Phi|\hat{A}|\Phi\rangle = \int \Phi^*(\vec{x})(\hat{A}\Phi)(\vec{x})\,\mathrm{d}\vec{x}$. Since $\langle\Phi|\Delta\hat{z}_j|\Phi\rangle = 0$, $j = 1, \ldots, 2n$, we have $\Delta_\alpha = 0$ for $|\alpha| = 1$.

Denote by $\hat{O}(\hbar^\nu)$ any operator $\hat{F}$ such that for any function $\Phi$, from the class $\mathcal{P}^t_\hbar(Z(t,\hbar))$, the asymptotic estimate holds

$$\frac{\|\hat{F}\Phi\|}{\|\Phi\|} = O(\hbar^\nu), \qquad \hbar \to 0.$$

(2) The following asymptotic formula holds,

$$\{\Delta\hat{z}\}^\alpha = \hat{O}(\hbar^{|\alpha|/2}), \qquad \alpha \in \mathbb{Z}^{2n}_+, \qquad \hbar \to 0, \tag{3.3}$$

in particular,

$$\Delta\hat{x}_k = \hat{O}(\hbar^{1/2}), \qquad \Delta\hat{p}_k = \hat{O}(\hbar^{1/2}), \qquad k = 1, \ldots, n. \tag{3.4}$$

(3) For functions $\Phi(\vec{x}, t, \hbar) \in \mathcal{P}^t_\hbar(Z(t,\hbar))$ the following limits hold,

$$\lim_{\hbar\to 0} \frac{1}{\|\Phi\|^2}|\Phi(\vec{x}, t, \hbar)|^2 = \delta(\vec{x} - \vec{X}(t,0)), \tag{3.5}$$

$$\lim_{\hbar\to 0} \frac{1}{\|\tilde{\Phi}\|^2}|\tilde{\Phi}(\vec{p}, t, \hbar)|^2 = \delta(\vec{p} - \vec{P}(t,0)), \tag{3.6}$$

where $\tilde{\Phi}(\vec{p}, t, \hbar) = F_{\hbar,\vec{x}\to\vec{p}}\Phi(\vec{x}, t, \hbar)$, and $F_{\hbar,\vec{x}\to\vec{p}}$ is the $\hbar^{-1}$-Fourier transform [3].

Denote by $\langle\hat{A}(t)\rangle_\Phi$ the mean value of a self-adjoint in $L_2\left(\mathbb{R}^n_x\right)$ operator $\hat{A}(t)$, $t \in \mathbb{R}$, calculated with respect to the function $\Phi(\vec{x}, t, \hbar) \in \mathcal{P}^t_\hbar$:

$$\langle\hat{A}(t,\hbar)\rangle_\Phi = \frac{1}{\|\Phi\|^2}\langle\Phi(\vec{x}, t, \hbar)|\hat{A}(t,\hbar)|\Phi(\vec{x}, t, \hbar)\rangle.$$

(4) For a function $\Phi(\vec{x}, t, \hbar) \in \mathcal{P}^t_\hbar(Z(t,\hbar))$ and an operator $\hat{A}(t,\hbar)$ with Weyl symbol $A(z, t, \hbar)$ satisfying the first inequality in assumption 1, the following equality holds:

$$\lim_{\hbar\to 0}\langle\hat{A}(t,\hbar)\rangle_\Phi = A(Z(t,0), t, 0). \tag{3.7}$$

The limiting nature of conditions (3.5), (3.6) and the asymptotic character of estimations (3.2)–(3.4) allows the construction of an approximate solution $\Psi^{\mathrm{as}} = \Psi^{\mathrm{as}}(\vec{x}, t, \hbar)$ of a Hartree-type equation for any finite time interval $[0, T]$ in the following sense:

$$\left[-\mathrm{i}\hbar\frac{\partial}{\partial t} + \hat{\mathcal{H}} + \varkappa\hat{V}(\Psi^{\mathrm{as}})\right]\Psi^{\mathrm{as}} = O(\hbar^q), \tag{3.8}$$

$$\Psi^{\mathrm{as}} \in \mathcal{P}^t_\hbar(Z(t,\hbar)), \qquad t \in [0, T], \tag{3.9}$$

where $O(\hbar^q)$ denotes a function $g^{(q)}(\vec{x}, t, \hbar)$, $q > 1$, which represents the error for equation (2.1) and obeys the estimate

$$\max_{0\leqslant t\leqslant T}\|g^{(q)}(\vec{x}, t, \hbar)\| = O(\hbar^q), \qquad \hbar \to 0. \tag{3.10}$$

Following [16] and having in mind properties (3.5), (3.6), we call the function $\Psi^{\rm as}(\vec{x},t,\hbar)$ in (3.8) a *semiclassically-concentrated solution* $(\mathrm{mod}\,\hbar^{\alpha})$ for the Hartree-type equation (2.1).

The function $\Psi^{\rm as}(\vec{x},t,\hbar)$ of the Hartree-type equation is a formal asymptotic solution evolving from the initial state $\Psi_0(\vec{x},\hbar)$, which is chosen in the class $\mathcal{P}^0_\hbar(z_0)$ of initial $(t=0)$ trajectory-coherent functions. More precisely, let $z_0=(\vec{p}_0,\vec{x}_0)$ be an arbitrary point of the phase space $\mathbb{R}^{2n}_{px}$; introduce first the class

$$\mathcal{P}^0(z_0)=\left\{\Psi:\Psi(\vec{x},\hbar)=\varphi_0\left(\frac{\vec{x}-\vec{x}_0}{\sqrt{\hbar}}\right)\,\exp\left\{\frac{\mathrm{i}}{\hbar}\langle\vec{p}_0,\vec{x}-\vec{x}_0\rangle\right\},\varphi_0(\vec{x})\in\mathcal{S}\left(\mathbb{R}^n_x\right)\right\}.$$

Now we define $\mathcal{P}^0_\hbar(z_0)$ as the class of formal series in powers $\hbar^{1/2}$,

$$\mathcal{P}^0_\hbar(z_0)=\left\{\psi:\psi(\vec{x},\hbar)=\sum_{k=0}^{\infty}\hbar^{k/2}\Psi_k(\vec{x},\hbar),\,\Psi_k\in\mathcal{P}^0(z_0)\right\},\tag{3.11}$$

similarly to the definition of $\mathcal{P}^t_\hbar(Z(t,\hbar))$, but there is no dependence on $t$ in functions belonging to $\mathcal{P}^0_\hbar(z_0)$. For the fixed-point trajectory $Z(t,\hbar)=z_0$, the class $\mathcal{P}^0_\hbar(z_0)$ can be considered as the subclass of $\mathcal{P}^t_\hbar(z_0)$ corresponding to time-independent functions $\varphi$ and $S(t,\hbar)\equiv 0$.

Two standard examples of the amplitude function for an initial state are a *Gaussian wave packet*

$$\varphi_0(\vec{\xi})=\mathrm{e}^{-\langle\vec{\xi},A\vec{\xi}\rangle/2}$$

and a *Fock state of a multi-dimensional oscillator*

$$\varphi_0(\vec{\xi})=\mathrm{e}^{\mathrm{i}\langle\vec{\xi},Q\vec{\xi}\rangle/2}H_\nu(\mathrm{Im}\,Q\vec{\xi}).$$

In the first example $A$ is a real, symmetric and positive definite $n\times n$ matrix. In the second case $Q$ is a complex, symmetric $n\times n$-matrix with a positive definite imaginary part $\mathrm{Im}Q$, and $\nu=(\nu_1,\ldots,\nu_n)$ is a multi-index of the multi-dimensional Hermite polynomial $H_\nu(\vec{\eta})$, $\vec{\eta}\in\mathbb{R}^n$ [48].

A construction of a semiclassically-concentrated solution $(\mathrm{mod}\,\hbar^{\alpha})$ of the problem (2.1) with initial condition from (3.11) is based on a solution of the Hamilton–Ehrenfest system, to which we turn our attention now.

## 4. Hamilton–Ehrenfest system of ordinary differential equations

Let symbols $\mathcal{H}(z)$, $V(z,w)$ satisfy assumption 1. Then operator $\mathcal{H}(\hat{z})$ (2.2) is self-adjoint with respect to the inner product $\langle\Psi|\Phi\rangle$ in $L_2\left(\mathbb{R}^n_x\right)$ and operator $V(\hat{z},\hat{w})$ (2.2) is self-adjoint in $L_2\left(\mathbb{R}^{2n}_{xy}\right)$. Thus the norm of the exact solutions of (2.1) is preserved by time evolution: $\|\Psi(t)\|=\|\Psi_0\|$ (more about existence and norm preservation of the solution see e.g. [58, §3.1]). The mean value $\langle\hat{A}(t)\rangle=\langle\hat{A}(t)\rangle_\Psi$ of an operator $\hat{A}(t)=A(\hat{z},t)$, calculated with respect to these solutions obeys

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}(t)\rangle=&\left\langle\frac{\partial\hat{A}(t)}{\partial t}\right\rangle+\frac{\mathrm{i}}{\hbar}\langle[\mathcal{H}(\hat{z}),\hat{A}(t)]\rangle\\&+\frac{\mathrm{i}\varkappa}{\hbar}\left\langle\int\mathrm{d}\vec{y}\Psi^*(\vec{y},t,\hbar)[V(\hat{z},\hat{w}),\hat{A}(\hat{z},t)]\Psi(\vec{y},t,\hbar)\right\rangle,\end{aligned}\tag{4.1}$$

as an implication of the Heisenberg equation for evolution of operators. Equation (4.1) is called the *Ehrenfest equation for operator* $\hat{A}(t)$ *and function* $\Psi(\vec{x},t,\hbar)$. Our choice of this terminology is justified by analogy with the linear case $(\varkappa=0)$ in which equation (2.1) becomes the Schrödinger equation, while equation (4.1) is the Ehrenfest equation [4].

To derive the Hamilton–Ehrenfest system from the Ehrenfest equation (4.1) we take for $\Psi$ a solution of the Hartree-type equation (2.1) in the class of trajectory-coherent functions, and for $\hat{A}$ operators $\hat{z} = (\hat{\vec{p}}, \hat{\vec{x}})$ and $\{\Delta\hat{z}\}^\alpha$ with Weyl symbols $\{\Delta z\}^\alpha$, $\alpha \in \mathbb{Z}^{2n}_+$, where

$$\Delta z = z - Z(t,\hbar), \qquad Z(t,\hbar) = \frac{1}{|\Psi(t)|^2}\langle\Psi(t)|\hat{z}|\Psi(t)\rangle. \tag{4.2}$$

We represent operators $\mathcal{H}(\hat{z},t)$ and $V(\hat{z},\hat{w},t)$ in the series form

$$\begin{gathered}\mathcal{H}(\hat{z}) = \mathcal{H}(Z(t,\hbar)) + \sum_{|\mu|=1}^{\infty}\frac{1}{\mu!}\mathcal{H}_\mu(Z(t,\hbar))\{\Delta\hat{z}\}^\mu,\\ \varkappa V(\hat{z},\hat{w}) = \varkappa V(Z(t,\hbar),Z(t,\hbar)) + \tilde{\varkappa}\sum_{|\nu|=1}^{\infty}\sum_{|\mu|=2}^{\infty}\frac{1}{\nu!\mu!}V_{\mu\nu}(Z(t,\hbar))\Delta_\mu\{\Delta\hat{z}\}^\nu,\\ \mathcal{H}_\mu(z) = \frac{\partial^{|\mu|}\mathcal{H}(z)}{\partial z^\mu}, \qquad V_{\mu\nu}(z) = \left.\frac{\partial^{|\mu+\nu|}V(z,w)}{\partial z^\mu\partial w^\nu}\right|_{w=z}, \qquad \mu,\nu\in\mathbb{Z}^{2n}_+,\end{gathered} \tag{4.3}$$

where $\Delta_\mu$ are defined in (3.2) with $\Phi = \Psi(t)$, and $\tilde{\varkappa}$ is defined below after equation (4.6). Thus to derive the system we need to evaluate commutators $[\hat{z}_k, \{\Delta\hat{z}\}^\mu]$ and $[\{\Delta\hat{z}\}^\nu, \{\Delta\hat{z}\}^\mu]$ for $k = 1,\dots,2n$ and $|\mu| \geqslant 1, |\nu| \geqslant 1$. This has been done in the linear case ($\varkappa = 0$) [16, 22–24]) using a composition formula for Weyl symbols [41, appendix]: the symbol $C(z)$ of the product $\hat{C} = \hat{A}\hat{B}$ of operators with symbols $A(z)$ and $B(z)$ is

$$C(z) = A\left(\overset{2}{z} + \frac{\mathrm{i}\hbar}{2}J\overset{1}{\frac{\partial}{\partial z}}\right)B(z) = B\left(\overset{2}{z} - \frac{\mathrm{i}\hbar}{2}J\overset{1}{\frac{\partial}{\partial z}}\right)A(z). \tag{4.4}$$

Here the number over an operator refers to the order of its action onto the target function. This way we obtain an infinite system of equations for $Z_k(t,\hbar)$, $k = 1,\dots,2n$, $\Delta_\alpha(t,\hbar)$, $\alpha\in\mathbb{Z}^{2n}_+$. Keeping only the moments up to order $N$ (i.e. $|\alpha| \leqslant N$) we obtain the following finite system of equations,

$$\begin{aligned}\dot{Z}_k &= \sum_{j=1}^{2n}\sum_{|\mu|=0}^{N}\frac{1}{\mu!}J_{kj}\left(\mathcal{H}_{j\mu}(Z)\Delta_\mu + \tilde{\varkappa}\sum_{|\nu|=0}^{N}\frac{1}{\nu!}V_{j\mu\nu}(Z)\Delta_\mu\Delta_\nu\right),\\ \dot{\Delta}_\alpha &= \sum_{|\mu+\gamma|=0}^{N}(-\mathrm{i}\hbar)^{|\gamma|-1}\frac{[(-1)^{|\gamma_p|}-(-1)^{|\gamma_x|}]\alpha!\theta(\alpha-\gamma)\theta(\mu-J\gamma)}{\gamma!(\alpha-\gamma)!(\mu-J\gamma)!2^{|\gamma|}}\\ &\quad\times\left(\mathcal{H}_\mu(Z) + \tilde{\varkappa}\sum_{|\nu|=0}^{N}\frac{1}{\nu!}V_{\mu\nu}(Z)\Delta_\nu\right)\Delta_{\alpha-\gamma+\mu-J\gamma} - \sum_{k=1}^{2n}\alpha_k\dot{Z}_k\Delta_{\alpha(k)}\end{aligned} \tag{4.5}$$

with initial conditions

$$Z|_{t=0} = z_0 = \frac{1}{|\psi|^2}\langle\psi|\hat{z}|\psi\rangle, \qquad \Delta_\alpha|_{t=0} = \frac{1}{|\psi|^2}\langle\psi|\{\hat{z}-z_0\}^\alpha|\psi\rangle, \qquad \alpha\in\mathbb{Z}^{2n}_+, \quad |\alpha|\leqslant N. \tag{4.6}$$

Here $\tilde{\varkappa} = \varkappa\|\psi(\vec{x},\hbar)\|^2$, and $\psi(\vec{x},\hbar)$ is an initial state from $\mathcal{P}^0_\hbar(z_0)$ (3.11),

$$\begin{gathered}\mathcal{H}_{j\mu}(Z) = \left.\frac{\partial^{|\mu|+1}\mathcal{H}(z)}{\partial z_j\partial z^\mu}\right|_{z=Z}, \qquad V_{j\mu\nu}(Z) = \left.\left(\frac{\partial^{|\mu+\nu|+1}V_z(z,w)}{\partial z_j\partial z^\mu\partial w^\nu}\right)\right|_{w=z=Z},\\ \alpha = (\alpha_p,\alpha_x), \qquad J\alpha = (\alpha_x,\alpha_p), \qquad \alpha(k) = (\alpha_1-\delta_{k1},\dots,\alpha_{2n}-\delta_{k,2n}),\end{gathered} \tag{4.7}$$

$\theta(\alpha-\beta)=\prod_{k=1}^{2n}\theta(\alpha_k-\beta_k)$, where $\theta(x)$ is the step function: $\theta(x)=1$ for $x\geqslant 0$, $\theta(x)=0$ for $x<0$. As in the linear case $\varkappa=0$ (see [16]), the system (4.5) will be called *the Hamilton–Ehrenfest system of order N*. Due to the estimates (3.2) this system is equivalent in the class of trajectory-coherent states to the Hartree-type equation (2.1) with accuracy $O(\hbar^{(N+1)/2})$.

Introduce notations

$$\mathfrak{H}(z,w)=\mathcal{H}(z)+\tilde{\varkappa}V(z,w),\qquad \mathfrak{H}_z(Z)=\mathfrak{H}_z(z,w)|_{w=z=Z}=\left\|\frac{\partial\mathfrak{H}(z,w)}{\partial z_j}\right|_{w=z=Z}\Bigg\|_{1\times 2n},$$

$$\mathfrak{H}_{zz}(Z)=\mathfrak{H}_{zz}(z,w)|_{w=z=Z}=\left\|\frac{\partial^2\mathfrak{H}(z,w)}{\partial z_j\partial z_k}\right|_{w=z=Z}\Bigg\|_{2n\times 2n}. \tag{4.8}$$

Then for $N=0$ the Hamilton–Ehrenfest system (4.5) has the form

$$\dot{Z}=J\mathfrak{H}_z(Z), \tag{4.9}$$

and for $N=2$ we obtain

$$\begin{cases}\dot{Z}=J\left[\partial_z\left(1+\frac{1}{2}\langle\partial_z,\Delta_2\partial_z\rangle+\frac{1}{2}\langle\partial_w,\Delta_2\partial_w\rangle\right)\mathfrak{H}(z,w)\right]\big|_{w=z=Z},\\ \dot{\Delta}_2=J\mathfrak{H}_{zz}(Z)\Delta_2-\Delta_2\mathfrak{H}_{zz}(Z)J,\qquad \Delta_2^{\mathsf{T}}=\Delta_2,\end{cases} \tag{4.10}$$

where $\Delta_2(t)$ is a symmetric $2n\times 2n$ matrix with components $\Delta_\alpha$, $\alpha\in\mathbb{Z}_+^{2n}$, $|\alpha|=2$,

$$(\Delta_2)_{ij}=\Delta_{(\delta_{i1}+\delta_{j1},\delta_{i2}+\delta_{j2},\ldots,\delta_{i,2n}+\delta_{j,2n})},\qquad i,j=1,\ldots,2n.$$

Note that the quantities $\{\Delta_\alpha\}$, $\alpha\in\mathbb{Z}_+^{2n}$ must satisfy an infinite system of inequalities[4] (generalized Heisenberg uncertainty conditions). Assuming, in addition, that $\Delta_\alpha$ at $t=0$ satisfy estimations (3.2), the initial conditions (4.6) for the system (4.5) can be formulated without mentioning $\psi$ at all. It is physically obvious but mathematically unclear that all generalized Heisenberg inequalities should be consistent with equations (4.5), i.e. preserved by the time evolution.

The uncertainty relation for second moments, relevant already to the Hamilton–Ehrenfest system (4.10) of order 2, reads that the matrix $\Delta_2(t)+\frac{i\hbar}{2}J$ must be non-negative [50] (see also [16, 51]).

The fact that a finite system of ordinary differential equations (4.5) models (in the above explained sense) the evolution described by equation (2.1) with precision $O(\hbar^{(N+1)/2})$, suggests that a Hartree-type equation might allow an approximate semiclassical interpretation in the frameworks of classical mechanics with a finite number of degrees of freedom. The number of degrees of freedom of such a mechanical system would grow with precision order $N$. A study of such classical systems of quantum origin by methods of the theory of ordinary differential equations constitutes a separate interesting direction of research [27, 28].

## 5. Hamilton–Ehrenfest system of order two

### *5.1. General solution of truncated system*

An analysis of the second-order Hamilton–Ehrenfest system (4.10) will suffice for construction of the semiclassical spectrum in the next section.

Let $\mathfrak{g}(t)=(Z(t),\Delta_2(t))$ denote a vector solution of the system (4.10) with initial condition $\mathfrak{g}(0)=\mathfrak{g}^0$. Following (4.6), let $\mathfrak{g}^0=\mathfrak{g}^0_\psi$ be a vector of quantum means of the

[4] For $|\alpha+\beta|\leqslant 4$ the inequalities are well known (see e.g. [51] and the bibliography there).

corresponding set of operators in a state $\psi$:

$$\begin{aligned} &\mathfrak{g}^0_\psi = (Z(0),\, \Delta_2(0)), \quad Z_j(0) = \frac{1}{|\psi|^2}\langle\psi|\hat{z}_j|\psi\rangle, \\ &(\Delta_2)_{kl}(0) = \frac{1}{2|\psi|^2}\langle\psi|(\Delta\hat{z}_k\Delta\hat{z}_l + \Delta\hat{z}_l\Delta\hat{z}_k)|\psi\rangle, \end{aligned} \tag{5.1}$$

where $j, k, l = 1, \ldots, 2n$. To reflect, if necessary, the dependence of the solution $\mathfrak{g}(t)$ on the function $\psi$ we use the subscript notation $\mathfrak{g}_\psi(t)$, meaning that $\mathfrak{g}_\psi(0) = \mathfrak{g}^0_\psi$. Let $\psi \in \mathcal{P}^0_\hbar(z_0)$. Then $\mathfrak{g}_\psi(t)$ depends also on $\hbar$ and we write

$$\mathfrak{g}_\psi(t,\hbar) = \big(Z\big(t,\hbar,\mathfrak{g}^0_\psi\big),\, \Delta_2\big(t,\hbar,\mathfrak{g}^0_\psi\big)\big), \qquad \mathfrak{g}_\psi(0,\hbar) = \mathfrak{g}^0_\psi. \tag{5.2}$$

Estimations (3.2) suggest that solutions to the Hamilton–Ehrenfest system are to be sought as formal power series

$$\mathfrak{g}(t,\hbar) = \mathfrak{g}^{(0)}(t,\hbar) + \hbar\mathfrak{g}^{(1)}(t,\hbar) + \cdots, \tag{5.3}$$

or, equivalently,

$$\begin{aligned} &Z(t) = Z^{(0)}(t) + \hbar Z^{(1)}(t) + \cdots, \\ &\Delta_2(t) = \Delta_2^{(0)}(t,\hbar) + \hbar\Delta_2^{(1)}(t,\hbar) + \cdots. \end{aligned} \tag{5.4}$$

Substituting (5.4) into system (4.10) and ignoring terms of order $O(\hbar^q)$, $q \geqslant 3/2$, due to estimations (3.2), we obtain equations for $Z^{(0)}$, $Z^{(1)}$ and $\Delta_2^{(0)}$ with precision $O(\hbar^{3/2})$

$$\begin{cases} \dot{Z}^{(0)} = J\mathfrak{H}_z(Z^{(0)}), \\ \dot{Z}^{(1)} = J\mathfrak{H}_{zz}(Z^{(0)})Z^{(1)} + F\left(Z^{(0)}, \Delta_2^{(0)}\right), \\ \dot{\Delta}_2^{(0)} = J\mathfrak{H}_{zz}(Z^{(0)})\Delta_2^{(0)} - \Delta_2^{(0)}\mathfrak{H}_{zz}(Z^{(0)})J. \end{cases} \tag{5.5}$$

Here

$$F(Z,\Delta_2) = \frac{1}{2\hbar}J\partial_z \mathrm{Sp}\{[\mathfrak{H}_{zz}(z,w) + \tilde{\varkappa}V_{ww}(z,w)]\Delta_2\}|_{w=z=Z}, \quad V_{ww} = \left\| \frac{\partial^2 V(z,w)}{\partial w_j \partial w_k} \right\|_{2n\times 2n}. \tag{5.6}$$

The first equation of system (5.5) coincides with (4.9) and is similar in the linear case to the Hamilton system of classical mechanics. However, in the nonlinear case ($\tilde{\varkappa} \neq 0$) the system generally is not Hamiltonian.

Consider the following linear Hamiltonian system of equations which will be referred to as the *pseudo-system-in-variations* for the solution $Z^{(0)}(t)$:

$$\dot{a}_k = J\mathfrak{H}_{zz}(Z^{(0)}(t))a_k, \qquad k = 1, \ldots, n. \tag{5.7}$$

The normalization conditions [9] for its $2n$-vector solutions $a_k$, compatible with the system (5.7) are assumed:

$$\{a_k(t), a_l(t)\} = \{a_k^*(t), a_l^*(t)\} = 0, \qquad \{a_k^*(t), a_l(t)\} = -2\mathrm{i}\delta_{kl}, \tag{5.8}$$

where $\{u, v\}$ is a skew-symmetric bilinear form in $\mathbb{C}^{2n}$

$$\{u, v\} = \langle Ju, v\rangle, \qquad J^\intercal = -J, \qquad u, v \in \mathbb{C}^{2n}, \qquad \langle u, v\rangle = \sum_{j=1}^{2n} u_j v_j.$$

If a solution $Z^{(0)}(t)$ as well as the set $a_k(t)$, $k = 1, \ldots, n$, satisfying (5.7), (5.8), are known, then the general solution of the two last equations in (5.5) has the form

$$Z^{(1)}(t) = \sum_{k=1}^{n} [b_k(t)a_k(t) + b_k^*(t)a_k^*(t)], \tag{5.9}$$

$$\Delta_2^{(0)}(t) = A(t)\mathcal{D}A^+(t), \tag{5.10}$$

where scalar functions $b_k(t)$ and the $2n \times 2n$-matrix $A(t)$ are as follows,

$$b_k(t) = -\frac{1}{2\mathrm{i}} \int_0^t \{a_k^*(t), \tilde{F}(t)\}\,\mathrm{d}t + b_k, \qquad \tilde{F}(t) = F\left(Z^{(0)}(t), \Delta_2^{(0)}(t)\right), \tag{5.11}$$

$$A(t) = (a_1(t), a_2(t), \ldots, a_n(t), a_1^*(t), a_2^*(t), \ldots, a_n^*(t)), \tag{5.12}$$

and $A^+ = (A^*)^\intercal$, where $A^*$ denotes the complex conjugate to $A$ matrix $(A^*)_{ij} = (A_{ij})^*$. Here $b_k$ are constants of integration, $\mathcal{D}$ is an arbitrary $2n \times 2n$ constant matrix and $F(z, \Delta_2)$ is defined in (5.6). Thus in this approximation the total solution is determined by solutions of the modified classical system (4.9) and pseudo-system-in-variations (5.7).

### *5.2. Special solutions relevant to the rest point analysis*

We will consider in more detail one special class of solutions of system (5.5), which we will need in the next section.

**Assumption 2.** *Let the first equation of system (5.5) have a rest point solution $Z^{(0)}(t) = z_0$. Let the symplectic $(2n \times 2n)$-matrix $J\mathfrak{H}_{zz}(z_0)$ evaluated at the rest point $z_0$ have $n$ distinct pure imaginary eigenvalues $\mathrm{i}\Omega_k$, $\Omega_k > 0$, $k = 1, \ldots, n$* (and *$n$ eigenvalues complex conjugate to them, $-\mathrm{i}\Omega_k$, $k = 1, \ldots, n$*).

In the linear theory, assumption 2 implies stability of the rest point $z_0$ in the linear approximation [9]. Under assumption 2, solutions of the pseudo-system-in-variation (5.7) have the form

$$a_k(t) = \exp(\mathrm{i}\Omega_k t)\, f_k, \qquad k = 1, \ldots, n, \tag{5.13}$$

where $f_k$ is the eigenvector of the matrix $J\mathfrak{H}_{zz}(Z^{(0)}(t))$, evaluated at the rest point $Z^{(0)}(t) = z_0$

$$J\mathfrak{H}_{zz}(z_0)\, f_k = \mathrm{i}\Omega_k f_k, \qquad \Omega_k \neq \Omega_j, \qquad j, k = 1, \ldots, n. \tag{5.14}$$

The eigenvectors $f_k, k = 1, \ldots, n$, are normalized, without loss of generality, by condition (5.8).

Using (5.13), formulae (5.9) and (5.10) with (5.6), (5.11), (5.12) become

$$\begin{aligned} Z^{(1)}(t) &= \sum_{k=1}^{n} \mathrm{Re}\big[\{f_k^*, \mathfrak{F}_k(t)\} f_k + b_k\, \mathrm{e}^{\mathrm{i}\Omega_k t} f_k\big], \qquad b_k = \mathrm{const} \\ \Delta_2^{(0)}(t) &= \sum_{j,l=1}^{n} \frac{1}{2}\big(f_j f_l^+ + f_j^* f_l^\intercal\big)\mathcal{D}_{jl}\, \mathrm{e}^{\mathrm{i}(\Omega_j - \Omega_l)t}, \qquad f_l^+ = (f_l^*)^\intercal, \quad \mathcal{D}_{jl} = \mathrm{const}. \end{aligned} \tag{5.15}$$

Here the $2n$-vector $\mathfrak{F}_k(t)$ is defined by the relation

$$\mathfrak{F}_k(t) = \frac{1}{2\hbar} J\partial_z\, \mathrm{Sp}\{[\mathfrak{H}_{zz}(z, w) + \tilde{\varkappa} V_{ww}(z, w)]\mathcal{F}_k(t)\}|_{w=z=z_0}, \tag{5.16}$$

where the $(2n \times 2n)$-matrix $\mathcal{F}_k(t)$ has the following form,

$$\mathcal{F}_k(t) = \sum_{j,l=1}^{n} \frac{1}{2(\Omega_k + \Omega_j - \Omega_l)} \left(f_j f_l^+ + f_j^* f_l^\intercal\right) \mathcal{D}_{jl}\, \mathrm{e}^{\mathrm{i}(\Omega_j - \Omega_l)t}. \tag{5.17}$$

The time-independent solutions of system (5.5) are found from (5.15) for the special choice of constants $b_k = 0$, $\mathcal{D}_{jl} = \mathcal{D}_l \delta_{jl}$, and are as follows:

$$\Delta_2 = \sum_{l=1}^{n} \frac{1}{2}\big(f_l f_l^+ + f_l^* f_l^{\intercal}\big)\mathcal{D}_l, \qquad Z^{(1)} = \sum_{k=1}^{n} \mathrm{Re}\big[\big\{f_k^*, \mathfrak{F}_k^{\nu}\big\} f_k\big], \tag{5.18}$$

Here vector $\mathfrak{F}_k$ is defined by (5.16) with

$$\mathcal{F}_k(t) = \mathcal{F}_k = \frac{1}{2\Omega_k} \sum_{j=1}^{n} \mathcal{D}_j\big(f_j f_j^+ + f_j^* f_j^{\intercal}\big), \qquad \mathcal{D}_j = \mathrm{const}. \tag{5.19}$$

Here $\mathcal{D}_j$, $j = 1, \ldots, n$, are arbitrary constants. Thus, under assumption 2, an $n$-parametric family of the rest points (5.18) of system (5.5) is found. In the next section we will construct a semiclassical spectral series associated with it.

## 6. Semiclassical spectrum corresponding to a rest point of the Hamilton–Ehrenfest system for quantum means

Consider the stationary problem

$$\widehat{\mathcal{H}}_{\varkappa}(\varphi_{\nu})\varphi_{\nu} = E_{\nu}\varphi_{\nu}, \qquad \varphi_{\nu} \in L_2\big(\mathbb{R}_x^n\big). \tag{6.1}$$

Here $\nu = (\nu_1, \ldots, \nu_n) \in \mathbb{Z}_+^n$ is a multi-index with non-negative components.

Define *formal semiclassical eigenvalue* $E_{\nu}$ as a number $E_{\nu}(\hbar)$ for which there exists a function $\varphi_{\nu}(x, \hbar)$ with $\|\varphi_{\nu}(x, \hbar)\| = O(\hbar^0)$, such that

$$\widehat{\mathcal{H}}_{\varkappa}(\varphi_{\nu})\varphi_{\nu} = E_{\nu}\varphi_{\nu} + O(\hbar^{3/2}), \qquad \nu \in \mathbb{Z}_+^n, \tag{6.2}$$

where $O(h^{3/2})$ denotes a function with $L_2$-norm bounded from above by $\mathrm{const} \cdot \hbar^{3/2}$. A countable set of formal semiclassical eigenvalues $\{E_{\nu}\}$, $\nu \in \mathbb{Z}_+^n$, will be called a *semiclassical spectral series*. In this section we construct a semiclassical spectral series using solutions of the Hamilton–Ehrenfest system (4.10) for quantum means. In fact, it is sufficient to work with system (5.5), and the vector function $\mathfrak{g}_{\psi}(t, \hbar)$ (5.2) can be written mod $\hbar^{3/2}$ as follows[5]:

$$\mathfrak{g}_{\psi}(t, \hbar) = \big(Z_{(1)}(t, \hbar), \Delta_2^{(0)}\big(t, \mathfrak{g}_{\psi}^0\big)\big), \qquad Z_{(1)}(t, \hbar) = Z^{(0)}(t) + \hbar Z^{(1)}(t). \tag{6.3}$$

Invariant manifolds of classical Hamiltonian systems are known to be important for classification of spectral series in the linear theory ($\varkappa = 0$) [10]. We attempt to construct the semiclassical spectral series (6.2) and use invariant manifolds of system (5.5) for classification of them. In the simplest case, the invariant set consists of a single rest point: $Z^{(0)} = z_0$, $Z^{(1)} = \mathrm{const}$, $\Delta_2^{(0)} = \mathrm{const}$, found in (5.18), (5.19). It follows from (5.5) that $Z^{(0)} = \mathrm{const}$ is a solution of the algebraic equation

$$\mathfrak{H}_z(Z^{(0)}) = \partial_z[\mathcal{H}(z) + \tilde{\varkappa} V(z, w)]|_{w=z=Z^{(0)}} = 0. \tag{6.4}$$

We identify such $Z^{(0)}$ with point $z_0$, which defines class $\mathcal{P}_{\hbar}^0(z_0)$ (3.11). The following semiclassical spectral series is constructed, assuming that all semiclassical eigenstates (6.2) $\varphi_{\nu}$ belong to $\mathcal{P}_{\hbar}^0(z_0)$ and the *ground state* $\varphi_0$ is a coherent (or squeezed) state, i.e. it minimizes the uncertainty relation [50, 51]. In fact, such states can be found in an explicit form (6.20), but we do not need it in our method.

[5] Throughout this section a claim that a certain equation holds mod $\hbar^{3/2}$ means that terms of order $\hbar^q$, $q \geqslant 3/2$, are ignored due to estimates like (3.2).

**Statement 6.1.** *Under assumption 2 (section 5.2) a semiclassical spectral series (6.2) of the Hartree-type operator can be found* (mod $\hbar^{3/2}$) *as*

$$E_\nu = \mathfrak{H}(z_0, z_0) + \hbar \sum_{k=1}^{n} \widetilde{\Omega}_k \left( \nu_k + \frac{1}{2} \right), \qquad \nu \in \mathbb{Z}_+^n, \tag{6.5}$$

*where* $\mathfrak{H}(z, w)$ *is defined in (4.8) and*

$$\widetilde{\Omega}_k = \Omega_k + \frac{\tilde{\varkappa}}{2} \langle f_k^*, V_{ww}(z_0, z_0) f_k \rangle + \mathrm{Re} \sum_{j=1}^{n} \frac{\tilde{\varkappa}}{2\Omega_j} \langle V_w(z_0, z_0), f_j \rangle \langle f_j^*, \partial_z \rangle \langle f_k^*, [\mathfrak{H}_{zz}(z, w) + \tilde{\varkappa} V_{ww}(z, w)] f_k \rangle|_{z=w=z_0}. \tag{6.6}$$

*Here vectors* $f_k, k{=}1, \dots, n$, *are from (5.14), matrix* $V_{ww}$ *from (5.6), and vector* $V_w = \partial_w V(z, w)$.

For $\nu = 0$ our result (6.5) agrees with results obtained in [52].

To prove the statement we will need two lemmas.

**Lemma 6.1.** *Under assumption 2 (section 5.2) a semiclassical spectral series (6.2) of the Hartree-type operator can be written* (mod $\hbar^{3/2}$) *as*

$$E_\nu = \mathfrak{H}(z_0, z_0) + \sum_{j=1}^{n} \widetilde{\Omega}_j \mathcal{D}_j^{(\nu)}, \tag{6.7}$$

*where* $\widetilde{\Omega}_j$ *is given by (6.6) and* $\mathcal{D}_j^{(\nu)}$ *are some* $\nu$*-dependent values.*

**Proof.** The energy level $E_\nu$ can be found with accuracy $O(\hbar^{3/2})$ from the mean value of $\hat{\mathcal{H}}_\varkappa$ in the stationary state $\varphi_\nu \in \mathcal{P}_\hbar^0(z_0)$ as follows,

$$E_\nu = \frac{1}{|\varphi_\nu|^2} \langle \varphi_\nu | \hat{\mathcal{H}}_\varkappa(\varphi_\nu) | \varphi_\nu \rangle = \mathfrak{H}_\varkappa^{(2)}(\mathfrak{g}_{\varphi_\nu}(\hbar)) + \tfrac{1}{2} \mathrm{Sp} \{ \mathfrak{H}_{zz}(z_0) \Delta_2^\nu \} + O(\hbar^{3/2}), \tag{6.8}$$

where $\mathfrak{H}_\varkappa^{(2)}$ is defined in (A.2) and $\Delta_2^\nu = \Delta_2^{(0)}(\mathfrak{g}_{\varphi_\nu}^0)$. In derivation of (6.8) the equality (6.4) was used.

Note that for a stationary state $\varphi_\nu$ the solution $\mathfrak{g}_{\varphi_\nu}(\hbar) = \left( z_0 + \hbar Z_\nu^{(1)}, \Delta_2^\nu \right)$ (6.3) is time-independent and is found from (5.18), (5.19), in which the arbitrary constants $\mathcal{D}_k$ are denoted by $\mathcal{D}_k^{(\nu)}$ in order to reflect their relation to $\varphi_\nu$. Substituting $\Delta_2^\nu$ (5.18) into (6.8) we get after some calculations using (5.14)

$$E_\nu = \mathfrak{H}_\varkappa^{(2)}(\mathfrak{g}_{\varphi_\nu}(\hbar)) + \sum_{k=1}^{n} \Omega_k \mathcal{D}_k^{(\nu)} + O(\hbar^{3/2}). \tag{6.9}$$

Now, using (6.4), re-expand $\mathfrak{H}_\varkappa^{(2)}\left(\mathfrak{g}_{\varphi_\nu}(\hbar)\right)$ in (6.9) and obtain mod $\hbar^{3/2}$

$$\mathfrak{H}_\varkappa^{(2)}\left(\mathfrak{g}_{\varphi_\nu}(\hbar)\right) = \mathfrak{H}(z_0, z_0) + \hbar\tilde{\varkappa} \left\langle V_w(z_0, z_0), Z_\nu^{(1)} \right\rangle + \frac{\tilde{\varkappa}}{2} \mathrm{Sp} \left\{ V_{ww}(z_0, z_0) \Delta_2^\nu \right\}.$$

From formula (5.18) for $\Delta_2^\nu$ we get $\mathrm{Sp}\{V_{ww}(z_0, z_0)\Delta_2^\nu\} = \langle f_k^*, V_{ww}(z_0, z_0) f_k \rangle \mathcal{D}_k^{(\nu)}$. From (5.6) and (5.15), using $Z_\nu^{(1)}$ (5.18) with $\mathfrak{F}_k^\nu$ (5.19), we find

$$\left\langle V_w(z_0, z_0), Z_1^{(\nu)} \right\rangle = \mathrm{Re} \sum_{k=1}^{n} \sum_{j=1}^{n} \frac{1}{2\Omega_j} \langle V_w(z, w), f_j \rangle \langle f_j^*, \partial_z \rangle \langle f_k^*, [\mathfrak{H}_{zz}(z, w) + \tilde{\varkappa} V_{ww}(z, w)]|_{z=w=z_0} f_k \rangle \mathcal{D}_k^{(\nu)}. \tag{6.10}$$

Finally, from (6.9) and (6.10) we get (6.7), (6.6), which completes the proof of the lemma. □

Now our goal is to determine the values $\mathcal{D}_j^{(v)}$ in (6.7).

The values $\mathcal{D}_k^{(0)}$ are chosen so that the state $\varphi_0$ minimizes the uncertainty condition. This idea is supported by physical models including the harmonic oscillator and the Coulomb potential [53, 54] (see [51] and references therein). As mentioned at the end of section 4, the matrix $\Delta_2 + \frac{i\hbar}{2} J$ is non-negative. Thus for any complex vector $v$ we have

$$\left\langle v^*, \left(\Delta_2 + \frac{i\hbar}{2} J\right) v \right\rangle \geqslant 0,$$

with equality corresponding to minimization of the uncertainty relation. Take $v = Jf_j$, $j = 1, \ldots, n$. Then, using (5.18) with $\mathcal{D} = \mathcal{D}^{(0)}$ and skew-orthogonality relations (5.8), which hold for vectors $f_k$ as well as for $a_k(t)$, we have $\mathcal{D}_j^{(0)} \geqslant \frac{\hbar}{2}$. So, choosing

$$\mathcal{D}_j^{(0)} = \frac{\hbar}{2}, \tag{6.11}$$

we minimize the uncertainty relation. Thus we find

$$E_0 = \mathfrak{H}(z_0, z_0) + \frac{\hbar}{2} \sum_{j=1}^{n} \widetilde{\Omega}_j. \tag{6.12}$$

To complete the proof of the statement we need to show that

$$\mathcal{D}_j^{(v)} = \mathcal{D}_j^{(0)} + \hbar v_j, \qquad j = 1, \ldots, n. \tag{6.13}$$

We first note that a time-dependent solution $\mathfrak{g}_\psi(t, \hbar)$ (6.3) with $Z^{(0)} = z_0$ and $Z^{(1)}(t)$, $\Delta_2(t)$ defined in (5.15)–(5.17) has a form of an almost periodic [49] vector function with $n$ frequencies $\Omega_1, \ldots, \Omega_n$. They have the structure

$$\mathfrak{g}_\psi(t, \hbar) = \sum_{|\mu| \leqslant 2} \mathfrak{g}_\mu(\hbar)\, \mathrm{e}^{i\omega_\mu t}, \qquad \omega_\mu = \sum_{j=1}^{n} \Omega_j \mu_j, \tag{6.14}$$

where $\mu = (\mu_1, \ldots, \mu_n)$, is a multi-index with integer components $\mu_j = 0, \pm 1$, and $|\mu|$ denotes the sum of the absolute values of vector's components.

Let us now introduce the vector of mean values evaluated mod $h^{3/2}$

$$\widetilde{\mathfrak{g}_\psi}(t, \hbar) = (\widetilde{Z}, \widetilde{\Delta}_2), \qquad \widetilde{Z}_j = \frac{1}{|\Psi^{\mathrm{as}}|} \langle \Psi^{\mathrm{as}} | \hat{z}_j | \Psi^{\mathrm{as}} \rangle,$$

$$(\widetilde{\Delta}_2)_{kl} = \frac{1}{2|\Psi^{\mathrm{as}}|^2} \langle \Psi^{\mathrm{as}} | (\Delta \hat{z}_k \Delta \hat{z}_l + \Delta \hat{z}_l \Delta \hat{z}_k) | \Psi^{\mathrm{as}} \rangle, \qquad \Delta \hat{z} = \hat{z} - z_0,$$

where $\Psi^{\mathrm{as}}(\vec{x}, t)$ is a semiclassically-concentrated (approximate in the sense of (3.8) with $q = 3/2$) solution of (2.1) with initial condition $\Psi^{\mathrm{as}}(\vec{x}, 0) = \psi \in \mathcal{P}_\hbar^0(z_0)$.

Note that $\widetilde{\mathfrak{g}_\psi}(0, \hbar) = \mathfrak{g}_\psi(0, \hbar) = \mathfrak{g}_\psi^0$ (5.1), and by their definitions, the vectors $\widetilde{\mathfrak{g}_\psi}(t, \hbar)$ and $\mathfrak{g}_\psi(t, \hbar)$ (6.3) describe mean values of the same set of operators with the same precision. The following lemma presents $\widetilde{\mathfrak{g}_\psi}(t, \hbar)$ as an almost periodic function, which allows us to juxtapose it with $\mathfrak{g}_\psi(t, \hbar)$ found in (6.14). The required relation (6.13) will follow from that comparison.

**Lemma 6.2.** *Let $\psi = \sum_v C_v \varphi_v$ be a linear combination of at least two semiclassical eigenfunctions $\varphi_v \in \mathcal{P}_\hbar^0(z_0)$ (6.2). Then*

$$\widetilde{\mathfrak{g}_\psi}(t, \hbar) = \sum_{v, v'} \mathfrak{g}_{vv'}(\hbar)\, \mathrm{e}^{i\omega_{vv'} t}, \tag{6.15}$$

*where*

$$\hbar\omega_{vv'} = E_v - E_{v'} + \frac{1}{t} S\big[\mathfrak{g}_{\varphi_v}(\hbar)\big] - \frac{1}{t} S\big[\mathfrak{g}_{\varphi_{v'}}(\hbar)\big], \qquad v, v' \in \mathbb{Z}_+^n, \tag{6.16}$$

*with $S[\mathfrak{g}_{\varphi_v}(\hbar)]$ defined in (A.1) and $\mathfrak{g}_{vv'}(\hbar)$ being some time-independent quantities.*

**Proof.** At the initial moment of time we have $\Psi^{\mathrm{as}}(\vec{x},0) = \psi = \sum_\nu C_\nu \varphi_\nu(\vec{x})$, where $\varphi_\nu \in \mathcal{P}^0_\hbar(z_0)$, $C_\nu$ are constants. Thus for $t > 0$ the solution can be represented in the form (see appendix A):

$$\Psi^{\mathrm{as}}(\vec{x},t) = \exp\Big(\frac{\mathrm{i}}{\hbar}S[\mathfrak{g}_\psi(t,\hbar)]\Big)\sum_\nu C_\nu \exp\Big(-\frac{\mathrm{i}}{\hbar}E_\nu t - \frac{\mathrm{i}}{\hbar}S\big[\mathfrak{g}_{\varphi_\nu}(\hbar)\big]\Big)\varphi_\nu(\vec{x}). \tag{6.17}$$

Using function $\Psi^{\mathrm{as}}(\vec{x},t)$ in this form for evaluation of the mean values $\widetilde{\mathfrak{g}_\psi}(t,\hbar)$ we get (6.15), (6.16), which completes the proof. □

If the same initial condition $\psi$ is chosen for $\widetilde{\mathfrak{g}}_\psi(t,\hbar)$ and $\mathfrak{g}_\psi(t,\hbar)$ and similar terms are identified in the sums (6.15) and (6.14), then equality $\mathfrak{g}_{\nu\nu'}(\hbar) = \mathfrak{g}_\mu(\hbar)$ would imply the equality of the phases: $\omega_{\nu\nu'} = \omega_\mu$. Since $\omega_{\nu\nu'} = -\omega_{\nu'\nu}$ is anti-symmetric (cf (6.16)), we set $\mu = \nu - \nu'$ and obtain

$$\omega_{\nu\nu'} = \sum_{j=1}^n \Omega_j(\nu_j - \nu'_j). \tag{6.18}$$

Now we simplify the right-hand side of the formula (6.16). Since $\mathfrak{g}_{\varphi_{\nu'}}(t,\hbar) = \big(z_0 + \hbar Z^{(1)}_{\nu}, \Delta^{\nu}_2\big)$ (6.3) is time-independent, we find from (A.1)

$$\frac{1}{t}S\big[\mathfrak{g}_{\varphi_\nu}(\hbar)\big] = -\mathfrak{H}^{(2)}_x\big(\mathfrak{g}_{\varphi_\nu}(\hbar)\big). \tag{6.19}$$

Substitute (6.9), (6.19) into (6.16) to find that mod $\hbar^{3/2}$

$$\hbar\omega_{\nu\nu'} = \sum_{j=1}^n \Omega_j\big(D^{(\nu)}_j - D^{(\nu')}_j\big).$$

From this equation along with (6.18) we conclude that $D^{(\nu)}_j - D^{(\nu')}_j = \hbar(\nu_j - \nu'_j)$ for all $j = 1,\dots,n$, and find $D^{(\nu)}_j$ in terms of an arbitrary value $D^{(0)}_j$ as desired in (6.13).

Now (6.5) follows from (6.7) and (6.13), (6.11). Thus statement 6.1 is proved.

Note that the explicit form of the semiclassical eigenfunctions $\varphi_\nu \in \mathcal{P}^0_\hbar(z_0)$ was never required in the derivation of the semiclassical spectrum $E_\nu$. In fact, the functions can be found using ideas of the complex WKB method [9] modified for the nonlinear case [36, 37]. For completeness of the exposition we give them here without a derivation (the derivation to be published elsewhere [55]). The formula also can be used for a constructive demonstration that $E_\nu$ found in this section together with $\varphi_\nu$ given (mod $\hbar^{3/2}$) below obey equation (6.2) with desired accuracy (cf (A.9)):

$$\varphi_\nu = \frac{N_\nu\, \mathrm{e}^{\mathrm{i}\Phi(\Delta x)/\hbar}}{\sqrt{\det C(z_0)}}H_\nu\left(\frac{\Delta x}{\sqrt{\hbar}}\right), \qquad \Phi(\Delta x) = \langle p_0, \Delta x\rangle + \langle \Delta x, BC^{-1}(z_0)\Delta x\rangle, \tag{6.20}$$

$\Delta x = x - x_0$.

Here $z_0 = (p_0, x_0)$, $N_\nu$ is a normalization constant, and $H_\nu$, $\nu \in \mathbb{Z}^n_+$, are the multi-dimensional Hermite polynomials; the $n \times n$-matrices $B$ and $C$ are composed of the $n$ eigenvectors $f_k$ (5.14) as columns. The property $\operatorname{Im} BC^{-1}(z_0) > 0$ ensures that the set of $\varphi_\nu$ is complete in the space $\mathcal{P}^0_\hbar(z_0)$ (see e.g. [13, 16]).

## 7. Examples of semiclassical spectrum calculation

In this section we illustrate the method described above with examples of a Hartree-type equation (2.1) whose linear part corresponds to an oscillator, while the potential in the

nonlinear part is Gaussian. First, we consider a three-dimensional oscillator in a constant magnetic field. From this more general case we deduce results for a simpler one-dimensional model.

*7.1. Oscillator in a constant magnetic field and Gaussian nonlinear potential.*

In this example $n = 3$; consequently, $\vec{p} = (p_1, p_2, p_3)$, $\vec{x} = (x_1, x_2, x_3)$. The linear part of the Hamiltonian in equation (2.1) has the form

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\vec{p}} - \frac{e}{c}\vec{A}(\vec{x})\right)^2 + \frac{k}{2}|\vec{x}|^2. \tag{7.1}$$

The external field in the operator (7.1) is a superposition of a constant magnetic field $\vec{H} = (0, 0, H)$ with vector potential $\vec{A} = \frac{1}{2}\vec{H} \times \vec{x}$ and a harmonic oscillator field with scalar potential $\frac{k}{2}|\vec{x}|^2$. The non-local operator $\hat{V}(\Psi)$ in (2.2) has the form

$$\hat{V}(\Psi) = \int_{\mathbb{R}^3} V(\vec{x}, \vec{y})|\Psi(\vec{y}, t)|^2 \,\mathrm{d}\vec{y}, \qquad V(\vec{x}, \vec{y}) = V_0 \exp\left[-\frac{|\vec{x} - \vec{y}|^2}{2\gamma^2}\right]. \tag{7.2}$$

Here $H$, $V_0$, $k$, $\gamma$, $e$, $c$ are real parameters of the model.

We will be using notations $\omega_H$, $\omega_0$ and $\omega_{\mathrm{nl}}$ for the cyclotron frequency, oscillator frequency and nonlinear frequency, respectively:

$$\omega_H = \frac{eH}{mc}, \qquad \omega_0 = \sqrt{\frac{k}{m}}, \qquad \omega_{\mathrm{nl}} = \sqrt{\frac{|\tilde{\varkappa} V_0|}{m\gamma^2}}, \tag{7.3}$$

where $\tilde{\varkappa} = \varkappa\|\Psi\|^2$. We also introduce

$$\omega_a = \omega_0\sqrt{1 + \left(\frac{\omega_H}{2\omega_0}\right)^2}. \tag{7.4}$$

To construct a solution $\Psi \in \mathcal{P}^t_\hbar(Z(t, \hbar))$ of equation (2.1), (7.1), (7.2), we take a phase-space trajectory $Z(t, \hbar) = (\vec{P}(t, \hbar), \vec{X}(t, \hbar))$ that obeys (1.4), (1.5). Using notations (4.8), we have

$$\mathcal{H}(Z) = \frac{1}{2m}\vec{P}^2 + \frac{m\omega_a^2}{2}\left(X_1^2 + X_2^2\right) + \frac{m\omega_0^2}{2}X_3^2 + \frac{\omega_H}{2}(P_1X_2 - P_2X_1); \tag{7.5}$$

$$\mathfrak{H}_z(Z) = \mathcal{H}_z(Z) = \begin{pmatrix} \frac{1}{m}P_1 + \frac{\omega_H}{2}X_2 \\ \frac{1}{m}P_2 - \frac{\omega_H}{2}X_1 \\ \frac{1}{m}P_3 \\ -\frac{\omega_H}{2}P_2 + m\omega_a^2X_1 \\ \frac{\omega_H}{2}P_1 + m\omega_a^2X_2 \\ m\omega_0^2X_3 \end{pmatrix}. \tag{7.6}$$

The matrix of the second derivatives becomes

$$\mathfrak{H}_{zz}(z) = \begin{pmatrix} \mathfrak{H}_{pp}(z) & \mathfrak{H}_{px}(z) \\ \mathfrak{H}_{xp}(z) & \mathfrak{H}_{xx}(z) \end{pmatrix}, \tag{7.7}$$

$$\mathfrak{H}_{pp}(z) = \left\|\mathfrak{H}_{p_kp_l}(z)\right\|_{3\times3} = \frac{1}{m}\mathbb{I}, \tag{7.8}$$

$$\mathfrak{H}_{xx}(z) = \left\|\mathfrak{H}_{x_kx_l}(z)\right\|_{3\times3} = \mathrm{diag}\left(m\left(\omega_a^2 - \eta\omega_{\mathrm{nl}}^2\right), m\left(\omega_a^2 - \eta\omega_{\mathrm{nl}}^2\right), m\left(\omega_0^2 - \eta\omega_{\mathrm{nl}}^2\right)\right), \tag{7.9}$$

$$\mathfrak{H}_{px}(z) = \left\|\mathfrak{H}_{p_k x_l}(z)\right\|_{3\times 3} = \begin{pmatrix} 0 & \frac{\omega_H}{2} & 0 \\ -\frac{\omega_H}{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{7.10}$$

Here $\eta = \operatorname{sign}(\tilde{x}V_0)$.

To find the spectrum corresponding to the Hamiltonian in (2.1) we need only bounded solutions of the Hamilton–Ehrenfest system. The first equation of system (5.5) describes $Z_0(t,\hbar)$ and can be integrated independently from the other equations of the system. The last equation of (5.5) describes the second moments $\Delta_2(t)$ and depends on the solution of the first one. Therefore we start with solving the first equation of (5.5). The simplest stationary solution is the zero solution

$$Z_0(\hbar) = (\vec{P}_0(\hbar), \vec{X}_0(\hbar))^{\intercal} = (0,0,0,0,0,0)^{\intercal}. \tag{7.11}$$

Then the corresponding eigenvalue problem (5.14) has solutions $\Omega_1 = \omega_+, \Omega_2 = \omega_-$, $\Omega_3 = \omega_s$, with the Ritz frequencies

$$\omega_+ = \sqrt{\omega_a^2 - \eta\omega_{\mathrm{nl}}^2} + \frac{\omega_H}{2}, \qquad \omega_- = \sqrt{\omega_a^2 - \eta\omega_{\mathrm{nl}}^2} - \frac{\omega_H}{2}, \qquad \omega_{\mathrm{s}} = \sqrt{\omega_0^2 - \eta\omega_{\mathrm{nl}}^2}.$$

The eigenvectors are

$$\begin{aligned} f_1 &= \frac{1}{\sqrt{2}}\left(g_0, \mathrm{i}g_0, 0, -\frac{\mathrm{i}}{g_0}, \frac{1}{g_0}, 0\right)^{\intercal}, \\ f_2 &= \frac{1}{\sqrt{2}}\left(g_0, -\mathrm{i}g_0, 0, -\frac{\mathrm{i}}{g_0}, -\frac{1}{g_0}, 0\right)^{\intercal}, \\ f_3 &= \left(0, 0, g_{\mathrm{s}}, 0, 0, -\frac{\mathrm{i}}{g_{\mathrm{s}}}\right)^{\intercal}. \end{aligned} \tag{7.12}$$

Here $g_0 = \sqrt{\frac{m}{2}(\omega_+ + \omega_-)}$, $g_{\mathrm{s}} = \sqrt{m\omega_{\mathrm{s}}}$. The solutions $a_j(t)$ of (5.7) are found by (5.13) and are normalized by condition (5.8). They form a matrix $A(t)$ (5.12), which we rewrite in the block form

$$A(t) = \begin{pmatrix} B(t) & B^*(t) \\ C(t) & C^*(t) \end{pmatrix}, \tag{7.13}$$

where matrices $B(t)$, $C(t)$ have the following form,

$$B(t) = \begin{pmatrix} \frac{g_0\,\mathrm{e}^{\mathrm{i}\omega_+ t}}{\sqrt{2}} & \frac{g_0\,\mathrm{e}^{\mathrm{i}\omega_- t}}{\sqrt{2}} & 0 \\ \frac{\mathrm{i}g_0\,\mathrm{e}^{\mathrm{i}\omega_+ t}}{\sqrt{2}} & \frac{-\mathrm{i}\,g_0\mathrm{e}^{\mathrm{i}\omega_- t}}{\sqrt{2}} & 0 \\ 0 & 0 & g_{\mathrm{s}}\,\mathrm{e}^{\mathrm{i}\omega_s t} \end{pmatrix}, \qquad C(t) = \begin{pmatrix} \frac{-\mathrm{i}\,\mathrm{e}^{\mathrm{i}\omega_+ t}}{\sqrt{2}g_0} & \frac{-\mathrm{i}\,\mathrm{e}^{\mathrm{i}\omega_- t}}{\sqrt{2}g_0} & 0 \\ \frac{\mathrm{e}^{\mathrm{i}\omega_+ t}}{\sqrt{2}g_0} & \frac{-\mathrm{e}^{\mathrm{i}\omega_- t}}{\sqrt{2}g_0} & 0 \\ 0 & 0 & \frac{-\mathrm{i}\,\mathrm{e}^{\mathrm{i}\omega_s t}}{g_{\mathrm{s}}} \end{pmatrix}.$$

Using (6.13), (6.11) and (5.10) we find a solution of the last equation of system (5.5) in the block form

$$\Delta_2(t) = \begin{pmatrix} \sigma_{pp}(t) & \sigma_{px}(t) \\ \sigma_{xp}(t) & \sigma_{xx}(t) \end{pmatrix}, \tag{7.14}$$

in terms of the blocks $B(t)$, $C(t)$ of the matrix $A(t)$ (7.13) as follows,

$$\begin{aligned} \sigma_{xx}(t) &= \frac{\hbar}{2}(C(t)D(\nu)C^{+}(t) + C^*(t)D(\nu)C^{\intercal}(t)), \\ \sigma_{pp}(t) &= \frac{\hbar}{2}(B(t)D(\nu)B^{+}(t) + B^*(t)D(\nu)B^{\intercal}(t)), \\ \sigma_{px}(t) &= \frac{\hbar}{2}(B(t)D(\nu)C^{+}(t) + B^*(t)D(\nu)C^{\intercal}(t)), \end{aligned}$$

where the diagonal matrix $D(\nu) = \mathrm{diag}(\nu_1 + 1/2, \nu_2 + 1/2, \nu_3 + 1/2)$, $\nu_1, \nu_2, \nu_3 = 0, 1, 2, \ldots$. Matrices $\sigma_{xx}, \sigma_{pp}$ are diagonal and their explicit form is as follows:

$$\sigma_{xx}(t) = \frac{\hbar}{m}\,\mathrm{diag}\left(\frac{\nu_1+\nu_2+1}{\omega_+ + \omega_-}, \frac{\nu_1+\nu_2+1}{\omega_+ + \omega_-}, \frac{2\nu_3+1}{2\omega_s}\right)$$

$$\sigma_{pp}(t) = \frac{\hbar m}{4}\,\mathrm{diag}((\omega_+ + \omega_-)(\nu_1+\nu_2+1), (\omega_+ + \omega_-)(\nu_1+\nu_2+1), 2\omega_s(2\nu_3+1)).$$

The non-zero elements of the matrix $\sigma_{xp}(t)$ are $\sigma_{p_1x_2}(t) = -\sigma_{p_2x_1} = \hbar(\nu_1 - \nu_2)/2$.

After substitution (7.12) into (6.5), (6.6) and taking into account that for $V$ defined by (7.2), the vector $V_w(z_0, z_0) = 0$, and the only non-zero elements of the $6\times 6$ matrix $V_{ww}(z_0, z_0)$ are $(V_{ww})_{jj} = -V_0/\gamma^2$ for $j = 4, 5, 6$, we obtain the energy spectrum $E_\nu$ of the Hamiltonian $\hat{\mathcal{H}}_\varkappa$ (2.1), (7.1), (7.2)

$$E_\nu = \varkappa V_0 + \hbar\left[\left(\omega_+ - \frac{\eta\omega_{\mathrm{nl}}^2}{\omega_+ + \omega_-}\right)\left(\nu_1 + \frac{1}{2}\right) + \left(\omega_- - \frac{\eta\omega_{\mathrm{nl}}^2}{\omega_+ + \omega_-}\right)\left(\nu_2 + \frac{1}{2}\right) + \left(\omega_s - \frac{\eta\omega_{\mathrm{nl}}^2}{2\omega_{\mathrm{s}}}\right)\left(\nu_3 + \frac{1}{2}\right)\right] + O(\hbar^{3/2}). \tag{7.15}$$

Note that in the case of zero magnetic field $H = 0$, a similar expression for spectrum was obtained in [40].

### 7.2. *One-dimensional case*

Consider equation (2.1) with linear operator $\hat{\mathcal{H}}(t)$ in the form

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{k}{2}x^2, \tag{7.16}$$

and the nonlinear operator $\hat{V}(\Psi(t))$ as follows,

$$\begin{aligned} &\hat{V}(\Psi(t))\Psi(x,t) = \int_{-\infty}^{+\infty} V(x,y)|\Psi(y,t)|^2 dy\Psi(x,t),\\ &V(x,y) = V_0 \exp\left[-\frac{(x-y)^2}{2\gamma^2}\right]. \end{aligned} \tag{7.17}$$

In the absence of a magnetic field ($H = 0$), the cyclotron frequency (7.3) is equal to zero ($\omega_H = 0$), and thus from (7.4) we find $\omega_a = \omega_0$. Then for the Ritz frequencies we have

$$\omega_+ = \omega_- = \omega_{\mathrm{s}} = \sqrt{\omega_0^2 - \eta\omega_{\mathrm{nl}}^2}.$$

The Hamilton–Ehrenfest system with accuracy $O(\hbar^{3/2})$ in the case of operators (7.17) has the form

$$\begin{cases} \dot{p} = -kx,\\ \dot{x} = \dfrac{p}{m}, \end{cases} \tag{7.18}$$

$$\begin{cases} \dot{\sigma}_{xx} = \dfrac{2}{m}\sigma_{xp},\\ \dot{\sigma}_{xp} = \dfrac{1}{m}\sigma_{pp} - m\omega_{\mathrm{s}}^2\sigma_{xx},\\ \dot{\sigma}_{pp} = -2m\omega_{\mathrm{s}}^2\sigma_{xp}. \end{cases} \tag{7.19}$$

As a stationary solution of subsystem (7.18) we take the zero solution

$$Z_0(\hbar) = (P_0(\hbar), X_0(\hbar))^\intercal = (0, 0)^\intercal, \tag{7.20}$$

In this case matrix $A(t)$ (7.13) of solutions of the pseudo-system-in-variations (5.7) is a $2 \times 2$-matrix whose scalar blocks $B(t)$ and $C(t)$ satisfy the equations

$$\dot{B} = -m\omega_s^2 C, \qquad \dot{C} = \frac{B}{m}. \tag{7.21}$$

Floquet solutions $a(t) = (B(t), C(t))^\intercal$ of the system in variations (7.21) normalized by condition $\langle a, J^\intercal a^* \rangle = 2i$, $J = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ can be written in the form

$$a(t) = \frac{\exp(\mathrm{i}\omega_s t)}{\sqrt{m\omega_s}} \begin{pmatrix} \mathrm{i}m\omega_s \\ 1 \end{pmatrix}.$$

Then for the energy spectrum $E_n$ of the Hartree-type equation (2.1), (7.16), (7.17) we obtain

$$E_n = \varkappa V_0 + \hbar \left( \omega_s - \frac{\eta \omega_{\mathrm{nl}}^2}{2\omega_s} \right) \left( n + \frac{1}{2} \right) + O(\hbar^{3/2}). \tag{7.22}$$

## 8. Concluding remarks

An approach to the problem of correspondence between classical and quantum models in the nonlinear case has significant differences from the one feasible in linear quantum mechanics. In the linear quantum case, a transition from quantum to classical system in Ehrenfest's sense requires a certain property of a quantum-mechanical solution, namely the function has to be trajectory-coherent (1.5). A state which does not obey this condition is considered to be essentially quantum, but one which obeys it is near-classical. For near-classical states, classical dynamics obtained in the limit $\hbar \to 0$ is defined by a classical Hamilton function and appears to be the same regardless whether the quantum solution is localized (at each moment of time) at a point, on a curve or on a surface. (Exact meaning of localization on a curve or surface is explained e.g. in [2, 3].)

For a Hartree-type equation the situation is different. Classical equations (1.10) (or (4.9)) are valid only for states concentrated near a point at each moment of time. These classical equations are distinct from those obtained in [56–59]. The latter are integro-differential equations which describe dynamics of the $n$-dimensional manifolds in the $2n$-dimensional phase space. It was shown that for Hartee-type equations an implementation of Born's approach leads to those integro-differential equations for characteristics of a non-local (Vlasov) equation, which describes evolution of the classical density matrix. (Recall that in the linear case, the classical density matrix obeys the local Liouville equation, whose characteristics are trajectories of classical mechanics.) Thus equations of dynamics for point objects are different from those for elongated objects in the case of Hartree-type models. A rigorous derivation of classical equations describing dynamics of $k$-dimensional objects ($0 < k < n$) in $2n$-dimensional phase space constitutes a separate open problem.

The Hamilton–Ehrenfest systems (4.5) are subject of mathematical interest independently of their quantum origin. Questions similar to those posed in the linear case, such as about their Poisson structure and stability of solutions (including stability with respect to the nonlinearity parameter $\varkappa$), can be addressed in a future study.

The first nontrivial Hamilton–Ehrenfest system from the family (4.5) is (4.10). As we have demonstrated, a rest point of system (4.10) gives rise to a semiclassical spectral series $(E_\nu)$, approximate in the sense that the pairs $(E_\nu, \varphi_\nu)$ (6.5), (6.20) satisfy (6.2). A question about its relation to the exact solution of (6.1) is not simple. In this regard we note that:

(1) In the special case of a Hartree-type equation with quadratic potentials [38, 39] our approach gives exact eigenvalues (6.5) of equation (6.1).
(2) Formula (6.5) in the limit $\varkappa \to 0$ yields the semiclassical spectrum of the corresponding linear problem ((2.1) with $\varkappa = 0$), and the numbers $E_\nu|_{\varkappa=0}$ approximate (with accuracy $O(h^{3/2})$) exact eigenvalues in the energy range where the linear operator has discrete spectrum [2, 3].
(3) In contrast to the linear case ($\varkappa = 0$), a method which would allow us to prove that the formal semiclassical spectrum $E_\nu$ (6.2) approximates exact spectrum (6.1) is not developed yet. In general setting (2.1), (2.2) even the problem of existence of simple discrete spectrum for nonlinear Hartree-type operator is open. Only for some special cases such as the case of self-consistent field (1.8) with potentials that possess radial symmetries (see e.g. [60]) the existence of spectral series was justified. Nevertheless, as one can see from (6.8), if there exists a countable set of exact eigenfunctions $\varphi_\nu$ such that all of them are from the space $\mathcal{P}^0_\hbar(z_0)$ and $\varphi_0$ is a coherent (squeezed) state, then (6.5) gives an approximation of the exact values $E_\nu$ with accuracy $O(\hbar^{3/2})$. We stress once again that an explicit formula for such functions $\varphi_\nu$ is not required.

In this paper we have shown how the semiclassical spectrum for a Hartree-type equation can be retrieved from the rest-point solution of the related Hamilton–Ehrenfest system. Similarly, other quantum characteristics, such as quasi-energy spectrum, geometric and adiabatic phases, can be reconstructed from solutions of corresponding Hamilton–Ehrenfest systems. We will attempt to demonstrate that in detail in future publications. Note that in our approach the quantum characteristics can be found without solving the quantum equation. This is particularly valuable and advantageous due to a lack of general methods for solving Hartree-type equations.

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## Appendix A

Introduce the generalized action [36, 37] along the trajectory $\mathfrak{g}_\psi(t,\hbar) = (Z_{(1)}(t,\hbar), \Delta_2^{(0)}(t))$ (6.3):

$$S[\mathfrak{g}_\psi(t,\hbar)] = \int_0^t \mathrm{d}t\Big[\Big\langle \vec{P}^{(0)}\big(t,\mathfrak{g}^0_\psi\big), \dot{\hat{X}}^{(0)}\big(t,\mathfrak{g}^0_\psi\big)\Big\rangle - \mathfrak{H}^{(2)}_\varkappa(\mathfrak{g}_\psi(t,\hbar))\Big], \tag{A.1}$$

where

$$\mathfrak{H}^{(2)}_\varkappa(\mathfrak{g}_\psi(t,\hbar)) = \mathfrak{H}(z,w)|_{w=z=Z_{(1)}(t,\hbar)} + \frac{\tilde{\varkappa}}{2}\mathrm{Sp}\Big\{V_{ww}(z,w)|_{w=z=Z^{(0)}(t)}\Delta_2^{(0)}\big(t,\mathfrak{g}^0_\psi\big)\Big\}. \tag{A.2}$$

Here $\mathfrak{H}(z,w)$ is defined in (4.8).

**Statement A.1.** *A solution $\Psi(\vec{x},t)$ of equation (2.1) with the same Hamiltonian as in (6.2) and initial condition $\Psi(\vec{x},0) = \psi = \sum_\nu C_\nu\varphi_\nu(\vec{x})$, may be written in the form (6.17). Here*

*$\{\varphi_\nu(\vec{x})\}_{|\nu|=0}^{\infty}$, $\varphi_\nu \in \mathcal{P}_\hbar^0(z_0)$, is a set of stationary trajectory-coherent states of equation (6.2), with corresponding eigenvalues $E_\nu$, and $S[\mathfrak{g}_\psi(t,\hbar)]$ is defined in (A.1).* □

This statement follows from the *nonlinear semiclassical superposition principle*, which we derive first.

**Lemma A.1.** *Let $\{\Psi_\nu(\vec{x},t)\}_{|\nu|=0}^{N}$ be a set of semiclassically-concentrated mod $\hbar^{3/2}$ solutions of equation (2.1) with initial conditions $\Psi_\nu(x,0) = \psi_\nu(\vec{x}) \in \mathcal{P}_\hbar^0(z_0)$. Then function*

$$\Psi(\vec{x},t) = \exp\left(\frac{\mathrm{i}}{\hbar}S[\mathfrak{g}_\psi(t,\hbar)]\right)\sum_{|\nu|=0}^{N} C_\nu \exp\left(-\frac{\mathrm{i}}{\hbar}S[\mathfrak{g}_{\psi_\nu}(t,\hbar)]\right)\Psi_\nu(\vec{x},t) + O(\hbar^{3/2}) \tag{A.3}$$

*also is a semiclassically-concentrated mod $\hbar^{3/2}$ solution of equation (2.1) with the initial condition $\Psi(\vec{x},0) = \psi(\vec{x}) = \sum_{|\nu|=0}^{N} C_\nu\psi_\nu(\vec{x}) \in \mathcal{P}_\hbar^0(z_0)$. Here notation (A.1) was used.*

**Proof.** Consider associated mod $\hbar^{3/2}$ to (2.1) the linearized in $\mathcal{P}_\hbar^t$ Schrödinger equation [36–39]

$$\left(-\mathrm{i}\hbar\frac{\partial}{\partial t} + \widehat{\mathfrak{H}}_0(\mathfrak{g}_\psi(t,\hbar))\right)\Psi = 0, \tag{A.4}$$

$$\widehat{\mathfrak{H}}_0(\mathfrak{g}_\psi(t,\hbar)) = \Big\{\mathfrak{H}(z,w) + \frac{\tilde{\varkappa}}{2}\mathrm{Sp}[V_{ww}(z,w)\Delta_2(t,\hbar)] + \langle\mathfrak{H}_z(z),\Delta\hat{z}\rangle + \frac{1}{2}\langle\Delta\hat{z},\mathfrak{H}_{zz}(z)\Delta\hat{z}\rangle\Big\}\Big|_{w=z=Z(t,\hbar)}, \qquad \Delta\hat{z} = \hat{z} - Z(t,\hbar). \tag{A.5}$$

Here $\mathfrak{g}_\psi(t,\hbar) = (Z(t,\hbar),\Delta_2(t,\hbar))$ is defined in (5.2), function $\mathfrak{H}(z,w)$, vector $\mathfrak{H}_z(z)$ and matrix $\mathfrak{H}_{zz}(z)$ are defined in (4.8). Substitute for the argument of $\widehat{\mathfrak{H}}_0(\mathfrak{g}_\psi(t,\hbar))$ (A.5) the expansion $\mathfrak{g}(t,\hbar) = \mathfrak{g}^{(0)}(t,\hbar) + \hbar\mathfrak{g}^{(1)}(t,\hbar)$ (5.3), where $Z^{(0)}(t)$ (5.4) is the principal term of the phase-space trajectory. Then with precision $O(\hbar^{3/2})$ we obtain

$$\widehat{\mathfrak{H}}_0(\mathfrak{g}_\psi(t,\hbar)) = \mathfrak{H}_\varkappa^{(2)}(\mathfrak{g}_\psi(t,\hbar)) + \langle\mathfrak{H}_z(Z^{(0)}(t)),\Delta\hat{z}_0\rangle + \tfrac{1}{2}\langle\Delta\hat{z}_0,\mathfrak{H}_{zz}(Z^{(0)}(t))\Delta\hat{z}_0\rangle, \tag{A.6}$$

where $\Delta\hat{z}_0 = \hat{z} - Z^{(0)}(t)$, and $\mathfrak{H}_\varkappa^{(2)}(\mathfrak{g}_\psi(t,\hbar))$ is defined in (A.2). □

A solution mod $\hbar^{3/2}$ of the equation (A.4) may be written in the form

$$\Psi(\vec{x},t;\mathfrak{g}_\psi(t,\hbar)) = \exp\left(\frac{\mathrm{i}}{\hbar}S[\mathfrak{g}_\psi(t,\hbar)]\right)\chi(\vec{x},t,Z^{(0)}(t)), \tag{A.7}$$

and the equation for $\chi(\vec{x},t,Z^{(0)}(t))$, taking into account (A.1), becomes

$$\begin{aligned}&\left(-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t} + \langle\dot{\bar{P}}^{(0)}(t),\Delta x_0\rangle + \frac{1}{2}\langle\Delta\hat{z}_0,\mathfrak{H}_{zz}(Z^{(0)}(t))\Delta\hat{z}_0\rangle\right)\chi = 0,\\ &\frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + \langle\dot{\bar{X}}^{(0)}(t),\nabla\rangle, \qquad \Delta x_0 = x - \vec{X}^{(0)}(t).\end{aligned} \tag{A.8}$$

Note that equation (A.8) is determined only by trajectory $Z^{(0)}(t)$ and is linear. For an initial state from class $\mathcal{P}_\hbar^0(z_0)$ with $z_0 = Z^{(0)}(0)$ we have

$$\chi = \frac{N\,\mathrm{e}^{\mathrm{i}\Phi(\Delta x)/\hbar}}{\sqrt{\det C(t)}}f\left(\frac{\Delta x}{\sqrt{\hbar}},t\right), \qquad \Phi(\Delta x) = \langle P^{(0)}(t),\Delta x\rangle + \langle\Delta x, BC^{-1}(t)\Delta x\rangle,$$

$$\Delta x = x - X^{(0)}(t). \tag{A.9}$$

Here $Z^{(0)}(t) = (P^{(0)}(t),X^{(0)}(t))$, $N$ is a normalization constant, function $f(\xi,t)$ is a polynomial in $\xi$ (in the simplest case $f = 1$); $n\times n$-matrices $B(t)$ and $C(t)$ are composed

from components of $n$ vectors $a_k$ (5.7), and property $\operatorname{Im} BC^{-1}(t) > 0$ ensures that functions $\Psi$ of the form (A.7) belong to the space $\mathcal{P}^t_\hbar(Z(t))$.

It follows from linearity that if the initial state is represented as a linear combination

$$\chi(\vec{x},0,z_0)=\sum_{|\nu|=0}^{N} C_\nu \chi_\nu(\vec{x},0,z_0), \qquad \chi_\nu(\vec{x},0,z_0)\in\mathcal{P}^0_\hbar(z_0), \tag{A.10}$$

then

$$\chi(\vec{x},t,Z^{(0)}(t))=\sum_{|\nu|=0}^{N} C_\nu \chi_\nu(\vec{x},t,Z^{(0)}(t))+O(\hbar^{3/2}). \tag{A.11}$$

Now, from (A.7) we have $\Psi\big(\vec{x},0;\mathfrak{g}^0_\psi\big)=\chi(\vec{x},0,z_0)$, and thus (A.10) can be written as

$$\Psi(\vec{x},0)=\sum_{|\nu|=0}^{N} C_\nu \Psi_\nu(\vec{x},0), \qquad \Psi_\nu(\vec{x},0)\in\mathcal{P}^0_\hbar(z_0). \tag{A.12}$$

To complete the proof of the lemma it remains to observe that, taking into account (A.7), equation (A.3) is equivalent to (A.11).

To justify statement A.1 we take

$$\Psi_\nu(\vec{x},t)=\exp\left[-\frac{\mathrm{i}}{\hbar}E_\nu t\right]\varphi_\nu(\vec{x},\hbar)$$

and observe that $\mathfrak{g}_{\psi_\nu}(t,\hbar)=\mathfrak{g}_{\varphi_\nu}(\hbar)$ is time-independent. Then from (A.3) we obtain (6.17).

## Appendix B

Here we derive the properties of the trajectory-coherent functions listed in section 3.

1. Proof of (3.2). Rewrite the Weyl symbol of the operator $\{\Delta\hat{z}\}^\alpha$ in the form

$$(\Delta z)^\alpha=(\Delta\vec{p})^{\alpha_p}(\Delta\vec{x})^{\alpha_x}, \quad (\alpha_p,\alpha_x)=\alpha.$$

Then, in accordance with (2.5), we obtain the following formula for the mean value $\sigma_\alpha(t,\hbar)$ of the operator $\{\Delta\hat{z}\}^\alpha$:

$$\sigma_\alpha(t,\hbar)=\langle\Phi|\{\Delta\hat{z}\}^\alpha|\Phi\rangle=\frac{1}{(2\pi\hbar)^n}\int_{\mathbb{R}^{3n}}\mathrm{d}\vec{x}\,\mathrm{d}\vec{y}\,\mathrm{d}\vec{p}\,\Phi^*(\vec{x},t,\hbar)$$
$$\times\exp\Big(\frac{\mathrm{i}}{\hbar}\langle\vec{x}-\vec{y},\vec{p}\rangle\Big)[\Delta\vec{p}]^{\alpha_p}\left(\frac{\Delta\vec{x}+\Delta\vec{y}}{2}\right)^{\alpha_x}\Phi(\vec{y},t,\hbar).$$

Here

$$\Delta\vec{y}=\vec{y}-\vec{X}(t,\hbar).$$

After a change of variables

$$\Delta\vec{x}=\sqrt{\hbar}\vec{\xi}, \qquad \Delta\vec{y}=\sqrt{\hbar}\vec{\zeta}, \qquad \Delta\vec{p}=\sqrt{\hbar}\vec{\omega}$$

and using the formula for function $\Phi(\vec{x},t,\hbar)$ from the class $\mathcal{P}^t_\hbar(Z(t,\hbar))$ (3.1), we find

$$\begin{aligned}\sigma_\alpha(t,\hbar)&=\frac{1}{(2\pi\hbar)^n}\hbar^{3n/2}\hbar^{|\alpha|/2}2^{-|\alpha_x|}\int_{\mathbb{R}^{3n}}\mathrm{d}\vec{\xi}\,\mathrm{d}\vec{\zeta}\,\mathrm{d}\vec{\omega}\varphi^*(\vec{\xi},t,\hbar)\\&\quad\times\exp\{\mathrm{i}\langle\vec{\xi}-\vec{\zeta},\vec{\omega}\rangle\}\vec{\omega}^{\alpha_p}(\vec{\xi}+\vec{\zeta})^{\alpha_x}\varphi(\vec{\zeta},t,\hbar)\\&=\hbar^{(n+|\alpha|)/2}M_\alpha(t,\hbar),\\\|\Phi\|^2&=\hbar^{n/2}\int_{\mathbb{R}^n}\mathrm{d}\vec{\xi}\varphi^*(\vec{\xi},t,\hbar)\varphi(\vec{\xi},t,\hbar)=\hbar^{n/2}M_0(t,\hbar).\end{aligned}$$

Recall that the function $\varphi(\vec{\xi}, t, \hbar)$ depends on $\sqrt{\hbar}$ regularly and $M_0(t,\hbar) > 0$. Therefore,

$$\Delta_\alpha(t,\hbar) = \frac{\sigma_\alpha(t,\hbar)}{\|\Phi\|^2} = \hbar^{|\alpha|/2}\frac{M_\alpha(t,\hbar)}{M_0(t,\hbar)} \leqslant \hbar^{|\alpha|/2}\max_{t\in[0,T]}\frac{M_\alpha(t,\hbar)}{M_0(t,\hbar)} = O(\hbar^{|\alpha|/2}).$$

2. Proof of (3.3) follows from the definition (3.1) of a trajectory-coherent function $\Phi(\vec{x}, t, \hbar) \in \mathcal{P}^t_\hbar$ and the estimations (3.2).

3. Proof of (3.5). Consider a function $\phi(\vec{x})$ from the Schwartz class $\mathcal{S}(\mathbb{R}^n)$. Then for any function $\Phi(\vec{x}, t, \hbar) \in \mathcal{P}^t_\hbar$ the integral

$$\left\langle \frac{|\Phi(t,\hbar)|^2}{\|\Phi(t,\hbar)\|^2}\middle|\phi\right\rangle = \frac{1}{\|\Phi(t,\hbar)\|^2}\int_{\mathbb{R}^n_x}\phi(\vec{x})|\Phi(\vec{x},t,\hbar)|^2\,\mathrm{d}\vec{x}$$
$$= \frac{1}{\|\varphi(t,\hbar)\|^2}\int_{\mathbb{R}^n_x}\phi(\vec{x})\left|\varphi\left(\frac{\Delta\vec{x}}{\sqrt{\hbar}}, t\right)\right|^2\mathrm{d}\vec{x}$$

after the change of variables $\vec{\xi} = \Delta\vec{x}/\sqrt{\hbar}$ becomes

$$\langle|\Phi(t,\hbar)|^2|\phi\rangle = \frac{\hbar^{n/2}}{\|\varphi(t,\hbar)\|^2}\int_{\mathbb{R}^n_\xi}\phi(\vec{X}(t,\hbar)+\sqrt{\hbar}\vec{\xi})|\varphi(\vec{\xi},t,\hbar)|^2\,\mathrm{d}\vec{\xi}.$$

Taking the limit $\hbar \to 0$ and using

$$\|\varphi(t,\hbar)\|^2 = \hbar^{n/2}\int_{\mathbb{R}^n_\xi}|\varphi(\vec{\xi},t,\hbar)|^2\,\mathrm{d}\vec{\xi},$$

where the function $\varphi(\vec{\xi}, t, \hbar)$ depends on $\sqrt{\hbar}$ regularly, we obtain the statement.

Proof of (3.6) is similar to the previous one if we note that the Fourier image of the function $\Phi(\vec{x}, t, \hbar) \in \mathcal{P}^t_\hbar$ can be represented in the form

$$\tilde{\Phi}(\vec{p},t,\hbar) = \exp\left\{\frac{\mathrm{i}}{\hbar}[S(t,\hbar) - \langle\vec{p}, \vec{X}(t,\hbar)\rangle]\right\}\tilde{\varphi}\left(\frac{\vec{p}-\vec{P}(t,\hbar)}{\sqrt{\hbar}}, t, \hbar\right),$$

where

$$\tilde{\varphi}(\vec{\omega},t,\hbar) = \frac{1}{(2\pi)^{n/2}}\int_{\mathbb{R}^n_\xi}\mathrm{e}^{-\mathrm{i}\langle\vec{\omega},\vec{\xi}\rangle}\varphi(\vec{\xi},t,\hbar)\,\mathrm{d}\xi.$$

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