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Extension of the R-Σ Method to Any Order

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I. Introduction

In recent papers, a theory has been proposed that leads to a set of two Newton-like equations describing the single-particle dynamics. The dynamical variables are the expectation value $\boldsymbol{x}$ of the wave function ψ and its dispersion $\boldsymbol{\sigma}$ [1],[2]. The equations inherently account for the Heinsenberg position-momentum uncertainty relation. The theory is part of an investigation that aims at consistently incorporating quantum corrections into the transport model, for applications to advanced solid-state devices. The task is carried out in two steps. The first one, which is of interest for the present paper, derives two equations in which the dynamics of the dispersion of the single-particle wave function is accounted for in addition to that of the expectation value of position. The model is founded on an approximate description of the wave function that eliminates the need of the Ehrenfest approximation. As the dynamical variables of the model are the position and dispersion of the particle, the resulting equations are also termed "R-Σ equations" [3] to remind the symbols by which such variables are usually indicated in the literature.

The starting point of the method is the observation that the particle's localization is provided at every time t by the squared modulus $|\psi(\boldsymbol{\xi}, t)|^2$. Non-normalizeable wave functions are not considered. Here, $\boldsymbol{\xi} \equiv (\xi_1, \xi_2, \xi_3)$ denotes the coordinates, while the symbol $\boldsymbol{x} \equiv (x_1, x_2, x_3)$ is reserved for the expectation value. As $|\psi|^2$ can be reconstructed from its moments [1], the knowledge of the time evolution of the moments provides that of $|\psi|^2$. In turn, the moments' dynamics is described by Newton-like equations, that lend themselves to a statistical extension. In this way, a set of transport equations coherently incorporating quantum features may be worked out [2].

II. Theory

The position and dispersion are first- and second-order moments of $|\psi|^2$. It is of interest to extend the model beyond the second order, to the purpose of improving the understanding of its formal aspects and extending its practical applicability. In this paper, the model will be worked out to any order. As the calculations are quite involved, the results will be presented with reference to the one-dimensional case only. Letting $V(\boldsymbol{\xi}, t)$ be the potential energy, m the particle mass, $\mathcal{P} = -j\hbar\, \mathrm{d}/\mathrm{d}\xi$ the momentum operator, and

$$\langle \xi^r \rangle = \int |\psi|^2 \xi^r \, \mathrm{d}\xi \qquad (1)$$

the r-th moment of $|\psi|^2$, $r = 0, 1, \ldots$, the Newton equation for $\langle \xi^r \rangle$ reads

$$m \frac{\mathrm{d}^2 \langle \xi^r \rangle}{\mathrm{d}t^2} = -r \int |\psi|^2 \, \xi^{r-1} \frac{\mathrm{d}V}{\mathrm{d}\xi} \, \mathrm{d}\xi + \\ + a_r \int |\mathcal{P}\psi|^2 \, \xi^{r-2} \, \mathrm{d}\xi - b_r \, \langle \xi^{r-4} \rangle \, , \qquad (2)$$

where the normalization condition $\int |\psi|^2 \, \mathrm{d}\xi = 1$ is assumed, and $a_r = r(r-1)/m$, $b_r = \hbar^2 r(r-1)(r-2)(r-3)/(4m)$. Equation (2) is found starting from the espression of the time derivative of the expectation value of a time-independent operator $\mathcal{A}$,

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle \mathcal{A} \rangle = \frac{j}{\hbar} \int \psi^* \, (\mathcal{H}\mathcal{A} - \mathcal{A}\mathcal{H}) \, \psi \, \mathrm{d}\xi \, , \qquad (3)$$

with $\mathcal{H} = \mathcal{P}^2/(2m) + V$ the Hamiltonian operator, and by systematically applying suitable commutation rules involving quantum operators. Unfortunately, the possible commutation rules of Quantum Mechanics are many, whereas those useful for the purpose at hand are fewer. They are

$$\xi^r \, \mathcal{P} - \mathcal{P} \, \xi^r = r \, j\hbar \, \xi^{r-1} \, , \qquad (4)$$

$$\mathcal{P}\mathcal{G}_r - \mathcal{G}_r \mathcal{P} = -rj\hbar \mathcal{G}_{r-1} \, . \qquad (5)$$

with $-j\hbar\mathcal{G}_r = m \, (\mathcal{H}\xi^r - \xi^r \mathcal{H})$.

III. Discussion

A remarkable feature of (2) is that the second term at the right hand side does not contribute unless $r \geq 2$, and the third term does not contribute unless $r \geq 4$. Note that the dimensions of (2) are energy $\times$ length^{r-2}. As expected, the case $r = 1$ provides the standard relation

$$m\,\frac{\mathrm{d}^2\langle\xi\rangle}{\mathrm{d}t^2} = -\int |\psi|^2\,\frac{\mathrm{d}V}{\mathrm{d}\xi}\,\mathrm{d}\xi \qquad (6)$$

which, after parametrizing $|\psi|^2$ as $\delta(\xi - x)$ with $x = \langle\xi\rangle$, yields the Ehrenfest approximation. Note that such a parametrization is equivalent to expanding $\mathrm{d}V/\mathrm{d}\xi$ into a Taylor series around $\xi = x$ and truncating the series to order zero. Instead, the expansion of $\mathrm{d}V/\mathrm{d}\xi$ to the second order (still with $r = 1$) yields, after letting $\sigma = \langle\xi^2\rangle - x^2$,

$$m\,\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -\frac{\mathrm{d}V}{\mathrm{d}\xi} - \frac{\sigma}{2}\,\frac{\mathrm{d}^3 V}{\mathrm{d}\xi^3}\,, \qquad (7)$$

namely, the first of the R-Σ equations [1].

For the case $r = 2$ it is useful to remind that $m\,\dot{x} = \langle\mathcal{P}\rangle$ and $\langle\mathcal{P}^2\rangle = (\Delta p)^2 + m^2\dot{x}^2$, with $(\Delta p)^2$ the momentum dispersion. In the second-order approximation of the R-Σ model, such a dispersion is replaced with $\hbar^2/(4\sigma)$ by assuming that ψ is a minimum-uncertainty wave function. Such an assumption may be viewed as the closure condition for the system of Newton equations built up by the first and second moment. Expanding $\xi\,\mathrm{d}V/\mathrm{d}\xi$ to the second order around x yields, after some manipulation,

$$m\,\frac{\mathrm{d}^2\sigma}{\mathrm{d}t^2} = \frac{\hbar^2}{2m\sigma} - 2\sigma\,\frac{\mathrm{d}^2 V}{\mathrm{d}\xi^2}\,, \qquad (8)$$

namely, the second of the R-Σ equations. About Eq. (8) it is worth adding that the factor 2 multiplying $\sigma\,\mathrm{d}^2V/\mathrm{d}x^2$ was missing in the corresponding equations of Refs. [1], [2], and [3]. However, none of the conclusions of such papers is affected, with the exception of the calculation of the frequency of σ in the harmonic-oscillator type of motion, which must be corrected by a factor $\sqrt{2}$.

It may be argued that using the moments of $|\psi|^2$ may eventually lead to canceling the information carried by the phase of the wave function. Actually this is not true. In fact, using the polar form $\psi = \alpha\,\exp(j\beta)$, $\alpha > 0$, one finds

$$g_r \doteq m\,\frac{\mathrm{d}\langle\xi^r\rangle}{\mathrm{d}t} = r\,\langle\xi^{r-1}\hbar\beta'\rangle\,, \qquad (9)$$

where the prime indicates the derivative with respect to ξ. In particular, the case $r = 1$ of (9) is equivalent to $m\,\dot{x} = \langle\mathcal{P}\rangle$. As a consequence, the phase β also enters the second term at the right hand side of (2). Another remark is that the external force $-\mathrm{d}V/\mathrm{d}\xi$ enters only the first term at the right hand side of (2), while the other two terms are determined by the form of the wave function alone. If the force is absent, the evolution of the wave function is determined by the initial condition only. It follows that in this case the dynamics of the moments is determined solely by the initial conditions, as it should be. No matter what the force is, the initial conditions are determined by calculating (1) and (9) at $t = 0$. As $|\psi|^2 = \alpha^2$, one notices that the initial condition for the moment is determined by the wave function's modulus, whereas that for the moment's velocity is determined by the phase.

To bring the model beyond the second order it is necessary to add, say, the equation for $r = 3$ and expand $\xi^{r-1}\,\mathrm{d}V/\mathrm{d}\xi$ in (2) to the extent of making the third-order moment $\langle\xi^3\rangle$ to appear. The same scheme applies to the higher moments. Evidently, for $r > 2$ the closure condition $(\Delta p)^2 = \hbar^2/(4\sigma)$ of the second-order case becomes less sensible, because the modulus of the minimum-uncertainty wave function is Gaussian, which makes the odd moments of order $r \geq 3$ to vanish due to symmetry. It follows that the closure condition must incorporate the moments of order higher than the second.

References

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