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History and Philosophy of Quantum Mechanics III: Semiclassical Approach

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Abstract:
For an intermediate region between the microscopic and the macroscopic domain, the semi-classical method is the standard approach in which quantum mechanical variables are mixed with classical variables in a frame of classical models. However, this semi-classical approach seems to have some fundamental conceptual difficulties due to the incommensurability of the physical variables from classical and quantum mechanics. Furthermore, semi-classical hybrid models are rather fixed in their physical scale of application; they cannot be easily scaled up or down to emphasize or favor either classical or quantum elements. Thus, these hybrid models lack internal flexibility of adjusting their domains of application.

1. Introduction

Between the microscopic and macroscopic domains, there exists an intermediate region called the mesoscale domain. Physicists and other scientists often call this intermediate mesoscale domain either semi-classical or quasi-quantum domain. In recent years, newly developed major research activities under the name of nano-science and -technology are particularly interested in this region. Here, classical mechanics with its well-defined parameters and concepts can still be effectively employed, but, at the same time, some of quantum mechanical effects can also play a role in the overall dynamical behavior.

In condensed matter physics, so-called "semi-classical methods" have long been standard methods in which quantum mechanical variables are simply forced to work with classical variables in a framework of classical models (e.g. Ashcroft and Mermin, 1976, Chapter 2 and 12). However, developing an effective semi-classical model still remains very challenging in contemporary condensed matter physics. Ironically, semi-classical approaches can be more complicated than full quantum mechanical ones. One of the fundamental difficulties in semi-classical methods lies in the fact that the standard quantum mechanics does not overlap with classical mechanics in its application of the physical domain. The physical variables from the two theories are often said to be "incommensurable," and the so-called "quantum leap" lies in the mesoscale region.

However, in Bohmian quantum mechanics, classical variables can be employed continuously from the classical domain to the quantum one with no apparent "quantum leap" in between. This can be done by adjusting the contribution from the quantum potential term through a series expansion of it. Therefore, under the Bohmian scheme, developing a separate hybrid method such as the semi-classical method is simply redundant.

2. The Nano World

The "nano world" involves objects with at least one dimension between 1 and 100 nanometers (nm). Interestingly, this domain remains relatively unexplored by the standard quantum mechanics, although it is thought to be a fundamental theory of physics applicable in all possible physical scales. There are small but obvious quantum effects in mesoscale domain. However, a direct application of quantum mechanics as well as a semiclassical method to handle those small quantum effects in this domain is still a major task of current research in condensed matter physics. Physicists often see quantum mechanics as more fundamental than classical mechanics (i.e. quantum mechanics should include classical mechanics as a special case of it), covering all possible physical domains from micro to macro world. In this respect, they also say that quantum mechanics converges to classical mechanics when the Planck constant approaches zero. However, since the Planck constant is not exactly zero (although very small in its magnitude), this claim seems to admit that quantum mechanics does not converge perfectly to classical mechanics. Some physicists including, for example, a Nobel Laureate, Anthony Leggett, actively investigate exactly where (and when) quantum mechanical superposition states cease to appear in the transition from the quantum to classical domain, thereby questioning the validity of quantum mechanics in the mesoscale domain.

In current nano-science and -technology, properly accommodating quantum phenomena and simultaneously preserving the practical efficiency of classical concepts have been big challenges, especially in developing a dynamical model (for example, an electron transport theory) of a mesoscale system. The conventional methods from quantum mechanics are conceptually vague to work with, but quantum phenomena do begin to play a major role in the intermediate size or mesoscale domain. Furthermore, often in this size domain, the number of particles involved is far more than a single atom but, at the same time, far less than a collection of molecules. This intermediate collection of particles poses another considerable challenge under the conventional numerical scheme based on the standard quantum mechanics, since "exact quantum mechanical computations for a system with more than four or five atoms are unfeasible" (S. Garashchuk at the University of South Carolina, in private communication). So, the issue of computational efficiency also becomes very important in developing workable models in this mesoscale size range.

Thus, in practice, many working scientists in the field try to set up hybrid or semiclassical models of quantum and classical mechanics. According to Bokulich (2008 p.104), "semiclassical mechanics can be broadly understood as the theoretical and experimental study of the interconnections between classical and quantum mechanics. More narrowly, it is a field that uses classical quantities to investigate, calculate, and even explain quantum phenomena. Its methods involve an unorthodox blending of quantum and classical ideas, such as a classical trajectory with an associated quantum phase"(p.104). This unorthodox method is also "often referred to as "putting quantum flesh on classical bones," where classical mechanics provides the skeletal framework on which quantum quantities are constructed"(p.104).

Bokulich's understanding of the primary motivations for semi-classical mechanics is as follows: "First, in many systems of physical interest, a full quantum calculation is cumbersome or even unfeasible. Second, even when a full quantum calculation is within reach, semi-classical methods can often provide intuitive physical insight into a problem, when the quantum solutions are opaque. And, third, semi-classical investigations can lead to the discovery of new physical phenomena that have been overlooked by fully quantum mechanical approaches"(p.104). She also offers three reasons why a semi-classical scheme is desirable (in a context of application for atoms such as helium). "First, the semi-classical treatments provide an *investigative tool*: semi-classical methods allow one to investigate physical domains that might not yet be accessible either experimentally or with a fully quantum mechanical approach. Second, they provide a *calculational tool*: semi-classical calculations, though far from trivial, can be less cumbersome than full quantum calculations. Finally, they provide an *interpretive tool*: semi-classical methods can offer physical insights into the structure of a problem, in a way that a fully quantum-mechanical approach might not "(p.112). She then finally summarizes three lessons for semi-classical mechanics, after reviewing her case studies (p.132). First, there is a variety of *quantum* phenomena for which semi-classical mechanics provides the appropriate theoretical framework. Second, these semi-classical methods and explanations involve a thorough hybridization of classical and quantum ideas combined in both empirically adequate and conceptually fruitful ways. Third, these classical structures are actually manifesting themselves in surprising ways in the quantum experiments. Thus, "this speaks to a much richer continuity of dynamical structure across classical and quantum mechanics than is usually recognized" (p.132).

Interestingly, all of these motivations and lessons for semi-classical mechanics emphasized by Bokulich are almost exactly the advantages the Bohmian quantum mechanical scheme is claimed to possess here. The reason why there is 'the continuity of dynamical structure across classical and quantum mechanics' could be very well explained (conceptually and consistently) by Bohmian realism and determinism. However, although endorsing the view that these electron trajectories are more than mere fictions or calculational devices, Bokulich fails to appreciate Bohmian realism, while recognizing, in a passing footnote (p.125), that "there are, of course, consistent interpretations of quantum mechanics, such as Bohm's hidden variable theory, in which electrons do follow definite trajectories." She makes the following points clear: "The full realist claim, that electrons in atoms *really are* following these definite classical trajectories, would amount to a rejection of modern quantum mechanics and a violation of Heisenberg's uncertainty principle"(p.124). It seems that she does not fully recognize the broad scopes (and logical consistency) of Bohmian classical determinism. It should be also noted that Bohmian quantum mechanics does not really require a separate semi-classical approach of combining quantum and classical mechanics. Bohmian quantum mechanics is continuously applicable in both quantum and classical realms by adjusting the contribution of the quantum potential in the dynamical equations of motion.

Instead, Bokulich ends up emphasizing 'the continuity of dynamical structure between classical and quantum mechanics,' but not in Bohmian context: "The fertility of using classical concepts to model quantum phenomena lies in the fact that there is a continuity of dynamical structure between classical and quantum mechanics, and it is this dynamical structure, common to both theories, which is manifesting itself in these semi-classical experiments. Although there is no particle following these classical closed and periodic orbits, these trajectories nonetheless legitimately model certain features of the quantum dynamics in the semi-classical regime"(p.139), and "the success of semi-classical methods in providing both calculational and theoretical insight suggests that there is a greater continuity of dynamical structure across these theories that is traditionally recognized"(p.156). Finally, claiming not to be a realist, she positions herself as a structural realist "by paying attention to the structural features of scientific theories, rather than the particular ontologies or theoretical claims"(p.165).

In retrospect, Bokulich's main arguments on a structural continuity are based on the *phenomenological* success of semi-classical experimental works, and then she goes on to take the trajectories of the semi-classical theories as a totally heuristic and 'fictional' device. However, it should be pointed out that while some of the semi-classical theories may be successful in their applications, these hybrid semi-classical models still have an intrinsic and conceptual arbitrariness in the ways they mix classical and quantum mechanical variables, forcing them work in a single package. While, as Bokulich claims, these semi-classical methods of combing both quantum and classical motion can be empirically adequate and conceptually fruitful, the hybrid theories often become less satisfactory on a smaller physical scale in which more quantum mechanical effects start to come into play, and there is no way to estimate correction-errors involved in the calculations due to the initial arbitrariness. Specifically, the way in which classical and quantum variables are mixed in a hybrid model rigidly determines the size of its applicable domain. In other words, those hybrid models are rather fixed in their physical scale of application; they cannot be easily scaled up or down to emphasize or favor either classical or quantum elements. Thus, these hybrid models lack internal flexibility of adjusting their domains of application, for example, through some kind of free parameters to easily control the models from outside; once constructed, it is impossible to adjust the way in which classical and quantum variables are mixed. In addition, some theoretically minded physicists are still significantly concerned about conceptual incommensurability (i.e. as Bokulich admits, particle trajectories are real in classical mechanics whereas they are fictional in quantum mechanics) that hybrid computational models ignore between classical and quantum variables.

3. Semiclassical Models

Here, two particular examples of the semi-classical models can be taken from a standard solid-state physics textbook by Ashcroft and Mermin (1976, Chapter 2 and 12). The first example is Sommerfeld's semi-classical, free-electron gas model and the second is a time-dependent, semi-classical model of electron dynamics.

Shortly after the discovery of the Pauli exclusion principle, Arnold Sommerfeld applied his semi-classical approach to the classical free electron gas model originally first developed by Paul Drude. This model is nothing more than a model of classical electron gas with the single modification that the electronic velocity distribution is taken to be the quantum Fermi-Dirac distribution rather than the classical Maxwell-Boltzmann distribution. In order to understand Sommerfeld's idea, the quantum theory of electron is needed as follows.

A single electron can be described by a wave function □(**r**). If the electron has no interactions, physicists make the so-called 'free electron approximation.' Thus, as shown below, no potential energy term appears in the time-independent Schrödinger equation with a level of energy ε :

$$-\frac{(h/2\pi)^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]\Psi(r)=-\frac{(h/2\pi)^2}{2m}\nabla^2\Psi(r)=\varepsilon\Psi(r)$$

A boundary condition imposed on this equation shall represent the confinement of the electron to the volume V. The time-honored choice is so-called the Born-von Karman boundary condition, with a cube of side $L=V^{1/3}$, such that:

Ψ(x,y,z + L) = Ψ(x,y,z),

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Ψ(x + L,y,z) = Ψ(x,y,z).

A solution to the above time-independent Schrödinger equation, neglecting the Born-von Karman boundary condition, can be the so-called 'plane wave solution' (we can check this by substituting this solution back to the Schrödinger equation);

$$\Psi_k(r)=\frac{1}{\sqrt{V}}e^{ik\cdot r}\text{, with energy }\varepsilon(k)=\frac{(h/2\pi)^2k^2}{2m},$$

where **r** and **k** are the position and wave vector of an electron. The normalization constant $\frac{1}{\sqrt{V}}$ is picked such that the probability of finding the electron somewhere in the whole volume V is unity. Here, also note now that $\Psi_k(r)$ is an eigenstate of the the momentum operator,

$$\hat{p}=-i\frac{h}{2\pi}\nabla=-i\frac{h}{2\pi}\frac{\partial}{\partial r}$$

with eigenvalue **p** = (*h/2π*) **k**, because

$$-i\frac{h}{2\pi}\frac{\partial}{\partial r}e^{ik\cdot r}=\frac{h}{2\pi}ke^{ik\cdot r}.$$

Then, velocity **v** = **p**/m becomes

$$v=\frac{(h/2\pi)k}{m}.$$

This shows the 'plane wave solution' $e^{ik\cdot r}$ is constant in any plane perpendicular to **k** since such planes are defined by the equation **k·r** = constant. It is also periodic along lines parallel to **k**, with wavelength

$$\lambda=\frac{2\pi}{k}$$

known as the de Broglie wavelength. Now, invoking the Born-von Karman boundary condition permits only certain discrete values of **k**, since

$$e^{ik_xL}=e^{ik_yL}=e^{ik_zL}=1.$$

The components of the allowed wave vector **k** must then be of the following quantized form as the main conclusion of this Sommerfeld model:

$$k_x=\frac{2\pi n_x}{L},\ k_y=\frac{2\pi n_y}{L},\ k_z=\frac{2\pi n_z}{L}\quad\text{where } n_x,\ n_y,\ n_z \text{ are integers.}$$

As shown so far, Sommerfeld's semi-classical free electron model is totally based on the solution of the *time-independent* Schrödinger equation. So, 'free electrons' in the models are not really free as in a usual sense because of the *time-independent* (or confined) physical status. Consequently, it should be noted that this semi-classical model does not provide a description of any *time-dependent* dynamical system since the *time-independent* Schrödinger equation itself do not provide any meanings on the *time-dependent* motion of actual particles. In this model, physical variables both in quantum and classical mechanics are simply forced to work together in a given model.

As the second example of the semi-classical method within the standard quantum mechanical formulation, a time-dependent semi-classical model of electron dynamics (Ashcroft and Mermin 1976, Chapter 12) can be designed. This model is supposed to predict how, in the absence of collisions, a position **r**, a wave vector **k** and a band index **n** of each electron evolve in the presence of externally applied electric and magnetic fields, given the energy of an electron in a band as a function of its wave vector. This model is already based upon a given knowledge of the 'band structure' of the metal, and says nothing about how to compute the band structure in the first place. The aim of the model is just to relate the band structure to the transport properties of electron dynamics with the following assumptions: (Ashcroft and Mermin 1976, p.218)

- The band index n is a constant of the motion. So, this semi-classical model ignores the possibility of interband transitions.
- The time evolution of the position and wave vector of an electron with band index n are determined by the semi-classical equation of motion for the classical free electron gas in the presence of external electric and magnetic fields E(r, t) and H(r, t).
- In thermal equilibrium the contribution to the overall electronic distribution from those electrons in the n^{th} band is given by the usual Fermi distribution.

As the assumptions indicate, the restrictions of the semi-classical method include: first, one can consider each band to contain a fixed number of electrons of a particular type (of the Fermi distribution). As a result, only a small number of bands (or carrier types, namely electrons or 'holes') need to be considered in the description of a real metal or semi-conductor. Second, the equations of motion within each band in the assumption [2] are the same as the one for a classical free electron. Then, in the limit of zero periodic potential the semi-classical model must break down, for in that limit the electron will be a classical free electron, and in a uniform electrical field a free electron can continually increase its kinetic energy at the expense of electrostatic potential energy. This shows the primary difficulty of the model, which comes from the inconsistency between the classical and the quantum physical variables, when those physical variables are arbitrarily forced to work together. Third, the so-called 'crystal momentum' ħ**k** in the equation of the motion is not the momentum of a 'Bloch electron' in which the rate of change of an electron's momentum is given by the total force on the electron as in the equation of motion. Fourth, there is no way to estimate possible calculation-errors involved in such a mixed model.

As such, there are numerous outstanding conceptual problems inside this transport theory that remain unresolved. However, in Bohmian quantum mechanics, all classical variables can be continuously applicable to the quantum domain with no apparent "quantum leap" in between, by adjusting the corresponding contribution from the quantum potential term through some series expansions of it. Especially, the incommensurability between classical and quantum variables is not a conceptual issue in semi-classical (and also both quantum and classical) domain; the two Bohmian interpretations both in the ontological and the hydro-dynamical versions can be formulated to be an effective genuine quantum mechanics with all those classical concepts intact.

4. References

1. Ashcroft, N. W. and N. D. Mermin 1976. Solid State Physics. New York: Thomson Learning, Inc.
2. Bokulich, A. 2008. Reexamining the Quantum-classical Relation–Beyond Reductionism and Pluralism. Cambridge: Cambridge University Press