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REGULAR PAPER

An interpretation of quantum foundations based on density functional theory and polymer self-consistent field theory

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Abstract The Feynman quantum-classical isomorphism between classical statistical mechanics in 3+1 dimensions and quantum statistical mechanics in 3 dimensions is used to connect classical polymer self-consistent field theory with quantum time-dependent density functional theory. This allows the theorems of density functional theory to relate non-relativistic quantum mechanics to a classical statistical mechanical derivation of polymer self-consistent field theory for ring polymers in a 4 dimensional thermal-space. One dynamic postulate is added to two static postulates which allows for a description of quantum physics from a 5 dimensional thermal-space-time ensemble perspective. A connection with aspects of classical field theory can be made in the classical limit.

Keywords Quantum foundations · Density functional theory · Self-consistent field theory · Polymers

Mathematics Subject Classification 81P99 · 82C10

1 Introduction

It has been known for almost 70 years that equilibrium properties of many body quantum systems can be calculated using classical statistical mechanics through an isomorphism between quantum theory and ring polymers. The mathematics of this isomorphism was presented by Feynman in 1953 [1–3], an explicit identification with ring polymers was made by Chandler and Wolynes in 1981 [4], and this ring polymer isomorphism now forms the basis of path integral simulations [5–10]. The idea is that in quantum statistical mechanics, the partition function for quantum particles is expressed in terms of path integrals weighted by thermal "trajectories" running from zero to $\beta = 1/k_B T$, where k_B is Boltzmann's constant and T is the temperature. Feynman derived his exact partition function by treating β as an imaginary time variable [2], and although he didn't identify the thermal trajectory with classical ring polymers at the time, this has since become standard practice [4,5]. In this context, "polymer", does not refer literally to a macromolecule, but rather to an extended, non-point-like contour. Actual polymers can be parametrized by a space-curve $\mathbf{r}(s)$ which gives the location in space $\mathbf{r}$ for a position s along the contour of the polymer. Quantum particles are parametrized by a thermal-curve $\mathbf{r}(s)$ which gives the expected location $\mathbf{r}$ in space

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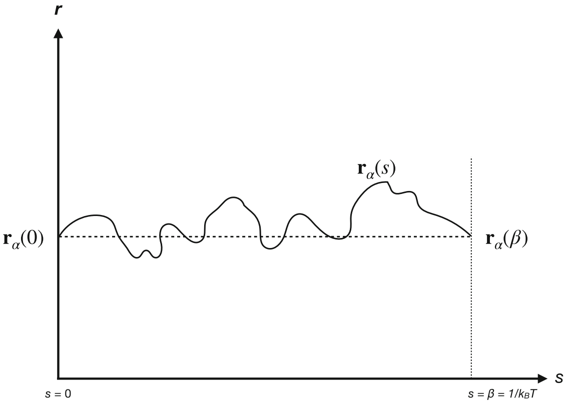

Fig. 1 Model of a quantum particle as a classical thread embedded in a four dimensional thermal-space. Three dimensional space is collapsed onto the y-axis and inverse thermal energy, $s = 1/k_BT$ is shown on the x-axis. One end of the quantum particle α starts at high classical temperature $s = 0$ at position $\mathbf{r}_\alpha(0)$, follows a thermal trajectory $\mathbf{r}_\alpha(s)$, and terminates at the same position $\mathbf{r}_\alpha(\beta) = \mathbf{r}_\alpha(0)$ at inverse thermal energy $\beta = 1/k_BT$

at an inverse temperature $s = \beta$. For quantum systems, one includes only trajectories for which $\mathbf{r}(0) = \mathbf{r}(\beta)$, so this maps onto ring polymers.

Another powerful tool for studying quantum many body systems is density functional theory (DFT). In previous work [11,12], it was shown that a theoretical polymer physics tool from equilibrium statistical mechanics called self-consistent field theory (SCFT), when applied to a system of ring polymers, gives identical mathematics as a quantum system in DFT. In other words, classical SCFT for ring polymers is isomorphic with quantum DFT. This is not surprising given the known isomorphism between classical and quantum partition functions just reviewed. An advantage of the SCFT perspective is that it is derived from first principles without using the theorems of DFT. These theorems basically state that there is a one-to-one mapping between the DFT representation of quantum systems in terms of one-body density functions and the underlying wave function representation [13–15]. This means that one can either use the postulates of quantum mechanics to arrive at a description of quantum particles that is equivalent to higher dimensional classical ring polymers, or, based on the mathematics of the first principles SCFT derivation, one can instead postulate directly that quantum particles are thermal contours in a classical four dimensional thermal-space, with the extra dimension being the inverse thermal energy β. The DFT theorems then guarantee that all predictions will be consistent with known quantum mechanics. One is thus replacing the usual set of wave function-based postulates with a smaller number of assumptions in the 4D classical statistical mechanics interpretation.

It's a difficult thing to measure the explanatory power of a theory based on counting postulates; there are normally about a half dozen postulates in non-relativistic quantum mechanics, but this number can be reduced depending on the presentation. For static, non-relativistic quantum mechanics, it was already shown that only two postulates are needed in the SCFT ring polymer derivation [11,12]. The first is that quantum particles are fractal Gaussian threads in four dimensions (for the time independent case) – see figure 1. This is equivalent to postulating the Heisenberg uncertainty relation in three dimensions [12]. The second postulate is that, for more than two threads, the contours have classical excluded volume in static 4D thermal-space. This assumption was shown to produce the correct shell structure for atoms expected from the Pauli exclusion principle, as shown in figure 2, and so is a 4D replacement for the exclusion principle in 3D [12]. Most standard introductions to quantum mechanics don't include the exclusion principle as an explicit postulate, but Kaplan [16] has demonstrated that it cannot be proven through ideas of indistinguishability as is often suggested. Thus, for the static case, the number of postulates is so significantly reduced by adopting a ring polymer picture of quantum particles that this is evidence for suggesting it has more explanatory power than other quantum interpretations. Additionally, since the ring polymer model arises within classical statistical mechanics (both postulates are entirely classical), it is necessarily an ensemble (statistical) interpretation, so there is no measurement problem (no collapse of a wavefunction). This feature of the ensemble interpretation has been exhaustively examined by Ballentine [17–19] and has wide support – see for example Bransden and Joachain [20], Aharonov [21], Popper [22], Blokhintsev [23] and Einstein [24]. The ring polymer model is more specific than the generic ensemble interpretation however, since what might be considered "hidden variables" are clearly identified as thermal correlations, that is, the conformational degrees of freedom of the nonlocal polymer in the higher dimensional space [12].

The aim of this paper is to show that the classical 4D thermal-space ring polymer model of static quantum mechanics is consistent with 5D thermal-space-time quantum physics. That is, predictions of time-dependent quantum mechanics can be shown to arise from a classical model of contours in a 5D thermal-space-time. This will be shown by introducing a third postulate and applying the Runge–Gross theorem [25] of time-dependent density functional theory (TDDFT). It then follows that the results of classical electromagnetism, namely Maxwell's equations, can be connected to these three postulates, reducing the number of foundational assumptions within physics more broadly. This link with electromagnetism is achieved through the ideas of Kaluza [26], since the thermal-space-time approach physically identifies a fifth dimension and has the "cylinder condition" of Kaluza built-in for the classical limit, as will be explained.

In Sect. 2, the static case is reviewed, including a brief summary of the SCFT derivation, a list of the SCFT equations and how they are used, and example results for the calculation of the electron densities of several atoms – hydrogen, helium, aluminum and argon. In Sect. 3 the dynamic case is connected to TDDFT through a third postulate and a result of the Keldysh formalism [27]. The Runge–Gross result is then used as a "must-go" theorem to prove that the polymer SCFT thread picture is consistent with predictions of time-dependent non-relativistic quantum mechanics. The 5D nature of the polymer picture is used in Sect. 4 to connect the three polymer-thread postulates to classical electromagnetism. Brief conclusions are given in Sect. 5.

2 Review of the static case

It is helpful to begin by reviewing the static case to build the physical picture. Quantum particles are modelled as classical extended thread-like objects that follow random walks (the Gaussian thread model of polymer SCFT [28]) with no other internal structure. They are embedded in a four dimensional thermal space and describe trajectories, or thermal world lines, that start at high temperatures and end at the temperature of interest such that the end spatial position is the same as the start position. Thus quantum particles form "ring polymers" in a 4D thermal-space – see figure 1. These threads interact in the usual ways, for example, in an atom or molecule electrons will feel Coulomb potentials due to nuclei and electron–electron interactions. Since the threads are classical, the exclusion principle cannot be incorporated in terms of quantum numbers. Instead, a classical excluded volume is postulated between threads, or allowing for spin, between pairs of threads. This has been shown to reproduce correct shell structure in atoms [12] and bonding in molecules [29]. These and other predictions follow from performing classical statistical mechanics on this Gaussian thread model of quantum particles following the methods of polymer SCFT. The derivation of SCFT equations for general polymers can be found in references [30–35] and for ring polymers specifically in reference [36]. Full derivations will not be repeated here, but the main points will be summarized.

From equilibrium statistical mechanics in the canonical ensemble with N quantum particles (polymer-like Gaussian threads) in a volume V at a temperature T, the configurational integral of the partition function will be

$$Z = \int \prod_{\alpha=1}^{N} \tilde{\mathcal{D}}\mathbf{r}_\alpha \delta[\mathbf{r}_\alpha(0) - \mathbf{r}_\alpha(\beta)] \exp\left\{-\beta U[\hat{n}]\right\} \tag{1}$$

with the momentum part of the partition function contributing only constant terms that can be ignored. In (1), the contour of quantum particle α is given by $\mathbf{r}_\alpha(s)$ as depicted in figure 1, where s runs from zero (a high classical temperature) to $\beta = 1/k_B T$. The potential U contains terms such as Coulomb potentials and the Pauli excluded volume between threads, and is written as a functional of a density operator [37,38]

$$\hat{n}(\mathbf{r},\beta)=\sum_{\alpha=1}^{N}\delta(\mathbf{r}-\mathbf{r}_\alpha(\beta)). \tag{2}$$

Details on the explicit form for $U[\hat{n}]$ for atomic systems can be found in appendix E of reference [11]. The Boltzmann factor of the potential U is summed over possible trajectories of all N quantum particles in the system, as expressed by the path integrals in (1). Since these paths are random walks, the path integral is weighted as [38]

$$\tilde{\mathcal{D}}\mathbf{r}_\alpha \equiv \mathcal{D}\mathbf{r}_\alpha P[\mathbf{r}_\alpha;0,\beta] \tag{3}$$

with the factor

$$P[\mathbf{r}_\alpha;s_1,s_2]\propto \exp\left\{-\frac{m}{2\hbar^2}\int_{s_1}^{s_2}ds\left|\frac{d\mathbf{r}_\alpha}{ds}\right|^2\right\}. \tag{4}$$

The derivation of this functional weight for random walks has been discussed at length by Freed [39] and Chandrasekhar [40]. Only random walk trajectories that return to their starting points $\mathbf{r}_\alpha(0)$ contribute to the partition function, and the Dirac delta functions in (1) enforce this. The prefactors m and $\hbar$ in (4) are the mass of a quantum particle and Planck's reduced constant, respectively. To keep the model classical and rigorously avoid assuming aspects of quantum mechanics, one should not reference Planck's constant at this stage – an unknown constant should be the prefactor. However comparison of the resulting SCFT equations with any single observation automatically sets the constant to $m/2\hbar^2$ universally. As will be shown in Eq. (9), the ratio of the square of Planck's constant to the quantum particle mass plays the role of a diffusion constant in a modified diffusion equation [30–35] and thus is an immutable property of the thread depicted in figure 1, so the theory has no free parameters, and no recourse to standard quantum mechanical derivations or postulates is required. Related to this, it is sometimes argued that a factorial $N!$ for the partition function in the canonical ensemble has a quantum origin [41], but as clarified by Frenkel [42], a quantum perspective is not required for this factor. Thus the present approach remains entirely classical, albeit in higher dimensions, and the complexities of exchange of indistinguishable particles is avoided.

The partition function (1) can be exactly transformed to field-based quantities using Hubbard–Stratonovich transformations following references [30–36]. The resulting iterated path integral partition function is solved using a saddle function approximation resulting from the first term of a functional Taylor series expansion [43]. This ultimately gives a free energy of [11,12]

$$F[n,w]=-\frac{N}{\beta}\ln Q(\beta)-\int d\mathbf{r}w(\mathbf{r},\beta)n(\mathbf{r},\beta)+U[n]. \tag{5}$$

This is a functional of the quantum particle density $n(\mathbf{r},\beta)$ and a field $w(\mathbf{r},\beta)$. $U[n]$ is the potential energy functional of the density and $Q(\beta)$ is a single particle partition function, defined below. Expressions for both the density and the field are obtained, following the general approach proposed by Kim et al. [36], by setting functional derivatives of (5) with respect to $n(\mathbf{r},\beta)$ and $w(\mathbf{r},\beta)$ equal to zero, as is required in the saddle function approximation, giving

$$n(\mathbf{r},\beta)=\frac{n_0}{Q(\beta)}q(\mathbf{r},\mathbf{r},\beta) \tag{6}$$

$$w(\mathbf{r},\beta)=\frac{\delta U[n]}{\delta n(\mathbf{r},\beta)} \tag{7}$$

where $n_0=N/V$ is the overall density. The single particle partition function is given by

$$Q(\beta)=\frac{1}{V}\int d\mathbf{r}q(\mathbf{r},\mathbf{r},\beta) \tag{8}$$

where a propagator $q(\mathbf{r}_0,\mathbf{r},\beta)$ is a solution to the modified diffusion equation

$$\frac{\partial q(\mathbf{r}_0,\mathbf{r},\beta)}{\partial\beta}=\mathcal{H}q(\mathbf{r}_0,\mathbf{r},\beta) \tag{9}$$

with

$$\mathcal{H} = \frac{\hbar^2}{2m}\nabla^2 - w(\mathbf{r}, \beta) \tag{10}$$

subject to the "initial" conditions

$$q(\mathbf{r}_0, \mathbf{r}, 0) = V\delta(\mathbf{r} - \mathbf{r}_0). \tag{11}$$

Note that the density in (6) is slightly different in form to that used for real polymers in SCFT, where one would integrate over all contour values of s from 0 to β to get the volume fraction of the polymer. In (6) we only want the density at the single value of $s = \beta$, so there is no contour integral. In other words, real polymer contours are embedded in three dimensions, whereas quantum particles extend into the inverse thermal dimension.

The set of Equations (6)–(11) can be solved when the potential $U[n]$, which describes the system, is given. For example, for an atomic system, $U[n]$ would include Coulomb terms for the ionic nucleus and electron-electron interactions and a Pauli term to enforce the exclusion principle. One can also include corrections to compensate for the saddle function approximation, electron self-interactions, the interacting quantum kinetic energy or correlations. These are usually incorporated into a so-called "exchange-correlation" term in DFT. One can alternatively obtain the same set of equations through quantum statistical mechanics, using the standard postulates of quantum mechanics, as shown in appendix A of reference [11] following the method of Kirkwood [44,45] as described by McQuarrie [46]. Thus the approach outlined here for the static case is not a replacement for quantum mechanics, but is rather a re-expression of quantum mechanics in one higher dimension that requires fewer postulates.

It is instructive to examine some examples so as to clarify the practical use of the equation set (6)–(11). Several results are shown in figure 2 for ground state electron densities ($\beta \to \infty$)[1] of hydrogen, helium, aluminum and argon, compared to the predictions of Hartree-Fock (HF) theory [47]. For simplicity, electron correlations are being ignored, although they would be straightforward to include in SCFT using the same approximations as in DFT. In the absence of correlations, SCFT should agree with HF to be "exact". The SCFT electron density for hydrogen agrees exactly with the known analytical result, and that of helium agrees exactly with HF. Aluminum and argon both show expected shell structure – deviations from HF densities come from approximations to the potential as described in reference [12]. The approach works well for all example atoms, including aluminum which is an open-shell, non-spherically symmetric atom. Even though aluminum and argon have non-trivial exchange contributions, the free energies of these two atoms from Eq. (5) agree with HF predictions for binding energies to within 1.5% and 0.2%, respectively [48]. Those of hydrogen and helium are essentially identical to HF ($\lesssim 10^{-6}\%$).

An atomic calculation, which for any practical case will use approximations, would proceed as follows. One defines the external potential as the ionic Coulomb attraction of the atom, treating the nucleus as a point. One takes an initial guess for the electron density $n(\mathbf{r}, \beta)$ at the temperature of interest. From this and the ionic potential, one can define the entire potential from Eq. (7) – a Hartree potential was used for the electron-electron interaction term, corrected for electron self-interactions using a modified Fermi-Amaldi pre-factor [49,50]. A Flory-Huggins-Edwards type delta function pseudo-potential [31–33,35,51] was used to represent excluded volume between different electron "threads" following the method described in reference [12] for the Pauli potential. With the field now known, the diffusion equation (9) can be solved for the propagator $q(\mathbf{r}_0, \mathbf{r}, \beta)$ subject to the initial condition (11). The single particle partition function (8) can now be found, and also the electron density $n(\mathbf{r}, \beta)$ from Eq. (6). The output electron density is used as input into the set of equations again until the input and output densities reach self-consistency. It is the self-consistent electron densities that are plotted in figure 2. The free energies for these structures can be found from Eq. (5). In principle, multiple self-consistent solutions for a given physical situation are possible, based on different initial guesses, but one can select the ground state by comparing the free energies, just as is done in polymer SCFT and Kohn-Sham DFT. In figure 2, for example, the input density guess for the self-consistent calculation of an atom with atomic number Z was taken to be the SCFT output density of the element with atomic number $Z - 1$. This provides one with a high confidence that the free energy is the global minimum. In practice, it is more efficient to solve Eqs. (6)–(11) spectrally, by expanding all functions of position in

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[1] In calculations, it was found that $\beta = 100$ was sufficient to approach the ground state with high accuracy.

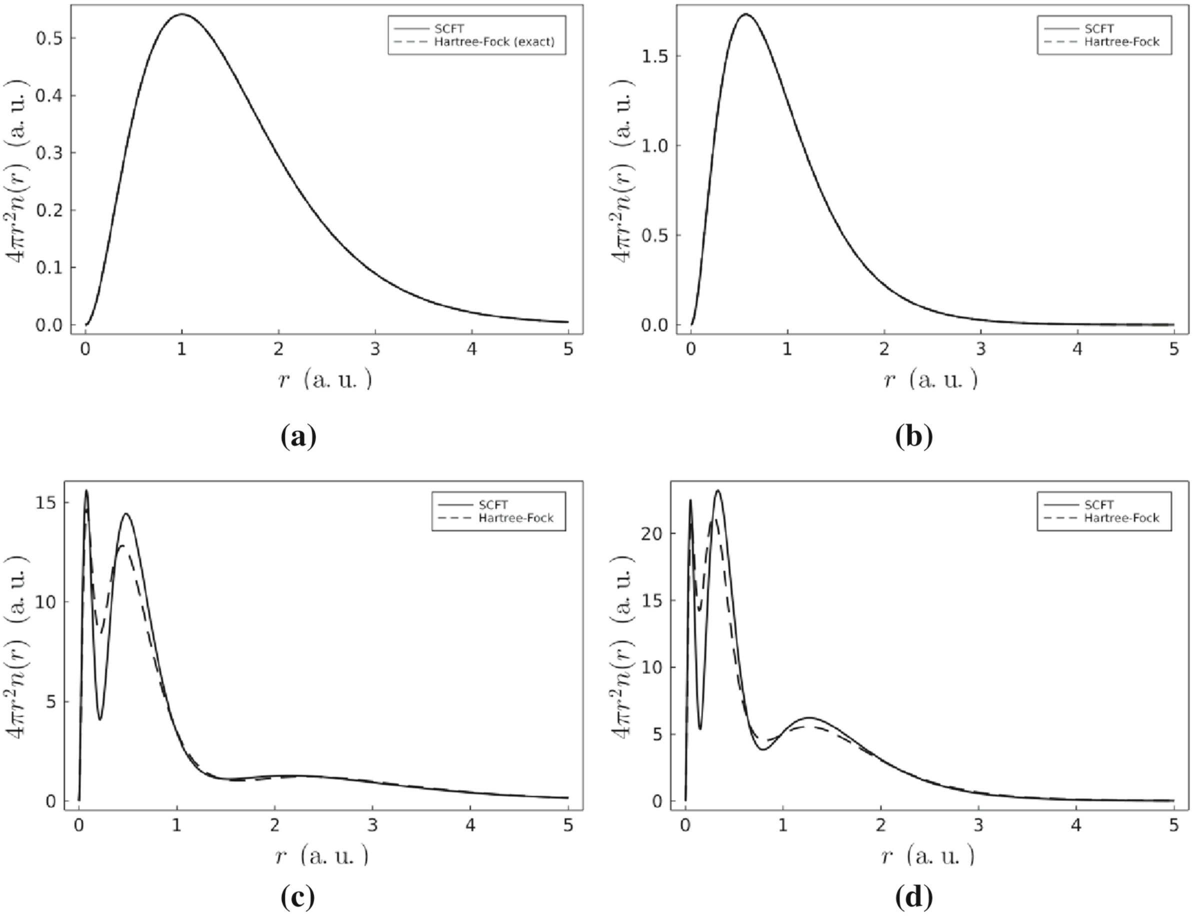

Fig. 2 Plot of ground state atomic radial electron densities as a function of radius, in Hartree atomic units, for (a) hydrogen, (b) helium, (c) aluminum and (d) argon, calculated using SCFT Eqs. (6)–(11)

a basis set that has the symmetry of the system. For example, in references [11,12], the case of isolated atoms was solved using spherical Bessel functions as the basis set. A Gaussian basis set was used for the electron densities in figure 2 [50]. The method can also be used to find the geometry of molecules by moving the ion centres, each time solving the electron density self-consistently, until the electronic free energy is minimized by the positions of the ions. In reference [29], the bond lengths and bond energies of a number of diatomic molecules were found using a basis set of Fourier series and cylindrical Bessel functions for the z and ρ directions, respectively. Since the Heisenberg uncertainty principle is built-in to the SCFT approach, being manifested in the extended thread nature of the particles, only the basis function set needs to be changed to consider different system symmetries.

Appendix B of reference [11] shows that the set of SCFT equations (6)–(11) reduces to Kohn-Sham DFT [52] assuming a perfect enforcement of the exclusion principle. This can be seen by finding the eigenvalues ε_i and eigenfunctions $\phi_i(\mathbf{r})$ of the operator $\mathcal{H}$ of Eq. (10), which are given by

$$\mathcal{H}\phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r}). \tag{12}$$

The modified diffusion equation (9) is then expanded in terms of the eigenfunctions of $\mathcal{H}$ so that the density (6) becomes [11,31]

$$n(\mathbf{r}) = \frac{1}{V} \sum_{i=1}^{\infty} f(\varepsilon_i - \mu)\, |\phi_i(\mathbf{r})|^2 \tag{13}$$

where $f(\varepsilon_i - \mu)$ is the Fermi-Dirac distribution and μ is the chemical potential. In the zero temperature limit, this becomes the familiar Kohn-Sham expression for the density.[2] Together with the Kohn-Sham Eq. (12) and an expression for the field $w(\mathbf{r}, \beta)$ from Eq. (7), the Kohn-Sham DFT equations are complete. The polymer thread SCFT picture is therefore equivalent to Kohn-Sham DFT, and so, through the theorems of DFT [13–15], the two postulates of the SCFT formalism are formally able to reproduce predictions of static, non-relativistic quantum physics from classical statistical mechanics in 4D.

3 Dynamic case

Quantum mechanics is fundamentally a dynamic theory. To incorporate dynamics into the SCFT methodology, one could use a direct generalization of the static derivation, although this "frontal assault" could be very difficult. It would involve a first principles non-equilibrium derivation of a dynamic action instead of a free energy. Then, one would vary the action to get a set of non-equilibrium equations describing quantum dynamics. One possible route for this could involve the Keldysh formalism [27]. Other possibilities from polymer physics are the dynamic partition function approach used by Grzetic, Wickham and Shi [53,54] and a similar method by Fredrickson and Orland [55]. Such methods still require postulating the dynamical behaviour of the thermal threads as input to the formalism and inevitably require many approximations. This is a familiar problem in polymer physics where dynamic generalizations of SCFT compromise conservation laws and often require working close to equilibrium — see for example references [53–61]. Whatever the method used, the results would need to be shown to reduce to a form of TDDFT so that the Runge–Gross theorem, which shows that a dynamic one-particle density can be used as the fundamental variable in quantum dynamics, would guarantee equivalent physical predictions to the wave function approach. This is the time-dependent version of the process used in the static case [11,12]. The frontal assault is only necessary however if one wants to find the time-dependent propagator corresponding to $q(\mathbf{r}_0, \mathbf{r}, \beta)$; one could call this unknown function $g(\mathbf{r}_0, \mathbf{r}, \beta, t)$. A formalism for finding $g(\mathbf{r}_0, \mathbf{r}, \beta, t)$ would be extremely useful; it would be the field-theoretic analogue of dynamic path integral simulation methods such as ring polymer molecular dynamics [6] and centroid molecular dynamics [7–10]. Other examples of representing quantum particle dynamics by classical polymer dynamics can be found in the references of Andersen [62]. It is not the objective of this work to present a formalism for such calculations, that is, a method for finding $g(\mathbf{r}_0, \mathbf{r}, \beta, t)$ will not be provided. Rather, the purpose here is to prove that it is *possible* to represent quantum dynamics in a field-theoretic way by a classical polymer model in five dimensions. This is in contrast to the simulation methods just mentioned which generally treat the extra thermal dimension as a mathematical tool without physical reality.

An alternative to deriving an expression for $g(\mathbf{r}_0, \mathbf{r}, \beta, t)$ is to postulate dynamics directly in terms of a time dependent density $n(\mathbf{r}, t)$, as illustrated in figure 3.

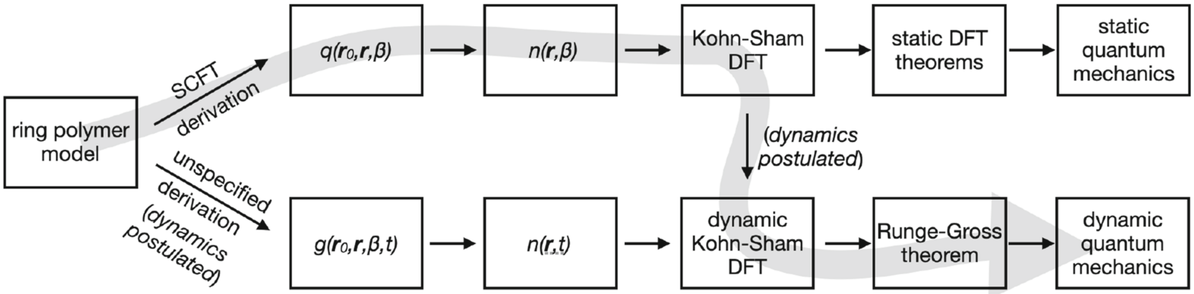

Fig. 3 A flowchart showing two different methods of connecting the ring polymer picture of quantum particles with time-dependent quantum mechanics. The method used in this article follows the grey arrow

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[2] The extra factor of $1/V$ is due to following the orthonormality definition of Matsen [31].

One can postulate the dynamic quantum particle density expression as the obvious generalization of Eq. (13):

$$n(\mathbf{r}, t) = \frac{1}{V} \sum_{i=1}^{\infty} f_i \, |\phi_i(\mathbf{r}, t)|^2 \tag{14}$$

where f_i is the occupancy at an initial time. Postulate (14) is incomplete without a definition for $\phi_i(\mathbf{r}, t)$, which is given by the time-dependent Kohn-Sham equation

$$i\hbar \frac{\partial}{\partial t} \phi_i(\mathbf{r}, t) = \mathcal{H} \phi_i(\mathbf{r}, t) \tag{15}$$

where $\mathcal{H}$ now has a time-dependent field

$$\mathcal{H} = \frac{\hbar^2}{2m} \nabla^2 - w(\mathbf{r}, t). \tag{16}$$

This time-dependent field would be specified according to the system under study. Eqs. (14)–(16) together form a complete mathematical statement of a single dynamical postulate.[3] This postulate conserves quantities such as mass, particle number, momentum, etc., and the equations are of the same form as Kohn-Sham TDDFT [63–65].[4] Just like in TDDFT, an exchange-correlation potential in $w(\mathbf{r}, t)$ will depend, in general, on the history of the time-dependent density $n(\mathbf{r}, t)$ and the initial state and so, in principle, memory effects are included in the formalism. In practice, memory effects are often ignored in TDDFT using the adiabatic approximation. Since Eqs. (14)–(16) are the same as in TDDFT, they will reproduce predictions of non-relativistic quantum mechanics through the theorem of Runge and Gross [25] and finite temperature generalizations [64,66] but from a five dimensional classical polymer model of quantum particles. This is the main point of this article. Rather than postulating the dynamical nature of the model and attempting to derive the mathematics, the mathematics have been postulated, and now all that is left is to verify that the postulated dynamics remain compatible with the classical ring polymer interpretation.

To this end, v-representability will be assumed for both TDDFT and static DFT throughout this work. The theorems of DFT guarantee a one-to-one mapping between a potential function v and a density function n. This means that given a Hamiltonian with a potential, there is a unique density that corresponds to it. Likewise, that density is generated *only* by that potential; no other potential (to within a spatially constant quantity) will give that same density function. However, an arbitrarily chosen density function does not necessarily correspond to *any* potential. Such a density is non-v-representable. Research into the mathematical foundations of DFT, including aspects of v-representability, is a large and important area — see references [67,68] for example for discussions of v-representability, ensemble v-representability, non-interacting v-representability, N-representability and density-potential mapping. These issues can be left beyond the scope of this work since, although a full proof of v-representability is still an open problem [68], it can be proven under fairly mild assumptions [63,69]. Quoting Ayer and Liu [70], "At this stage the authors view the problem as solved, albeit perhaps not completely understood." From a practical perspective, the assumption of v-representability for both TDDFT and static DFT is reasonable.

Many actual calculations using (14)–(16) exist — all of Kohn-Sham TDDFT is evidence of the practicality of these expressions [71]. The equations would be solved in a way similar to that described for the static case. An initial guess for the time and space evolution of the density $n(\mathbf{r}, t)$ is chosen. This is used to calculate a time dependent potential from the time dependent version of Eq. (7). The potential is used in (16) to solve the time-dependent Kohn-Sham Eq. (15), and the "orbitals" $\phi_i(\mathbf{r}, t)$ from this are used to find the time-dependent density (14) for $n(\mathbf{r}, t)$. As in the static case, this process is repeated until self-consistency between the input and output densities is achieved. TDDFT is used, for example, in studies of absorption spectra and photochemistry [71].

None of the results of TDDFT can be taken necessarily as evidence for a 5D classical polymer model of quantum particles since TDDFT is typically derived through other means [27].[5] The dynamic postulate (14)–(16) can be

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[3] One could include spin explicitly in the equations, or use time-dependent current density functional theory, but these features would unnecessarily complicate the presentation.

[4] It is assumed that the temperature is fixed throughout the dynamics, but that can be relaxed following reference [66].

[5] Since TDDFT by itself is not proof of the polymer thread model of quantum particles, no example of the application of Eqs. (14)–(16) is given in this text. One can refer instead to many applications of TDDFT in the literature – see for example [71] and references therein.

viewed as a phenomenological expression of the dynamics, and one needs to confirm that it is consistent with the original microscopic polymer-thread picture rigorously derived for the static case. The postulate (14)–(16) is consistent in the static limit with the classical model of thermal threads since (14)–(16) are constructed to reduce correctly to the static case. This is a necessary, but not sufficient condition for compatibility. It is also required that stationary, equilibrium points, of a dynamical trajectory are not special cases, with the polymer model applying only to those points.

The polymeric nature of the static model is captured by the modified diffusion equation (9) which statistically expresses the polymer degrees of freedom through the real-valued propagator $q(\mathbf{r}_0, \mathbf{r}, \beta)$. The static density is proportional to this quantity through Eq. (6), that is, $n(\mathbf{r}, \beta) \propto q(\mathbf{r}, \mathbf{r}, \beta)$. For the polymer model to be dynamically consistent with Eqs. (14)–(16), there should exist a real-valued time-dependent propagator $g(\mathbf{r}_0, \mathbf{r}, \beta, t)$ that is proportional to the time-dependent density, $n(\mathbf{r}, t) \propto g(\mathbf{r}, \mathbf{r}, t)$. From the Keldysh formalism [27], such a propagator is known to exist for the set of Eqs. (14)–(16).[6] Therefore the 5D classical ring polymer model of quantum particles is compatible with the postulated dynamics (14)–(16), which are in turn identical to the equations of TDDFT. So, through the Runge–Gross theorem, predictions of dynamic quantum mechanics are compatible with a 5D classical ring polymer model arising from only three postulates. Due to the non-local nature of the polymer-like threads, there is no conflict with Bell's theorems [72]. More generally, this approach is immune to other "no-go" theorems since it is rigorously shown to connect with DFT. The various theorems of DFT in effect act as "must-go" theorems, guaranteeing the equivalence of predictions between DFT (the classical thread picture) and quantum mechanics.

4 Electromagnetism

The three postulates given here also function to eliminate other assumptions that are external to quantum physics. The postulates require that there are five dimensions: three spatial, one temporal and one thermal. In the classical limit however, it has been proven that the ring polymer equations reduce to *classical* DFT – see appendix C of reference [11]. In other words, particles become point-like, shrinking to lose their contour aspects, and no longer depend on the fifth thermal dimension.[7] In the classical limit, the thermal dimension still exists, but no quantum quantities depend on it any longer. This is called a cylinder condition. A five dimensional classical theory subject to a cylinder condition derived following the methods of general relativity was published by Theodor Kaluza a century ago [26]. In what is known as the "Kaluza miracle", this theory spontaneously produced both Maxwell's equations of electromagnetism and 4D general relativity from 5D vacuum relativity equations [73]. It has been criticized for not identifying the fifth dimension nor justifying the cylinder condition [73]. As discussed in this article, the ring polymer interpretation of quantum foundations is five dimensional, with the fifth dimension clearly identified, and in the classical limit the cylinder condition automatically emerges. It is thus a "non-compactified" theory in which the cylinder condition is approximately true in the classical limit [73].

Other authors have suggested treating quantum particles as extended objects using completely different mathematics [62,74]. In particular, the approach of Andersen [62] uses quantum field theory rather than DFT, but is still based on a filament that exists in a physically real fifth dimension arising from Feynman's path integral expression of the partition function. Andersen is able to develop a perturbation theory in Feynman diagrams and show the development of loops and vacuum contributions once they are integrated over the fifth dimension. However alternative postulates to quantum mechanics are not given and the cylinder condition does not spontaneously emerge as it does in the DFT approach, so the relation with electrodynamics through the Kaluza idea is not as immediate.

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[6] See equations 3.12 and 3.13 of reference [27].

[7] Expression C7 of reference [11] can be seen to be a functional of only the density and not the field. In other words, in the classical limit, the polymer conformational degrees of freedom disappear (the polymer becomes like a point) on the relevant energy scales. In contrast, equation 17 of reference [11] must have the field $w(\mathbf{r})$ to account for the connectivity of the "segments" of the extended polymer - it does not behave like a point, and the conformational degrees of freedom in the excess entropy are identified to be the quantum kinetic energy of the "particle".

The connection with classical electrodynamics and a geometric picture of physics highlights a limitation in the DFT approach – there is a disconnect with the standard model which is based on quantum field theory. This could perhaps be partially alleviated through relativistic DFT, for which there is another existence theorem, analogous to the theorems of non-relativistic DFT, relating the one-particle density to quantum electrodynamics [75]. One could therefore consider replacing the time-dependent Kohn-Sham equation dynamical postulate with the Dirac-Kohn-Sham equation[8] while maintaining the physical interpretation of quantum particles as threads in 5D. This doesn't help more broadly with electroweak or strong interactions, nor does the DFT approach help in any way with quantum gravity. Also, while spin can be easily included in calculations within the SCFT formalism, a physical interpretation of spin, consistent with the extended thread picture of quantum particles, is not attempted, although there is some scope for this following the ideas of Belinfante [76] as described by Ohanian [77]. These issues are all beyond the scope of this article and are mentioned only to underline limitations of the ring polymer SCFT interpretation which is confined solely to non-relativistic quantum mechanics.

5 Conclusion

In summary, a classical ring polymer interpretation of quantum physics can reduce the number of postulates for quantum mechanics to three. It connects classical polymer SCFT with quantum DFT, making it consistent with Feynman's quantum-classical isomorphism and modern path integral simulation methods. The ensemble nature of the approach avoids the measurement problem, and there is a connection with classical electrodynamics through the ideas of Kaluza. Since the theory fits within classical statistical mechanics with an extra thermal dimension, there is improved economy of thought, and improved explanatory power. This recommends the 5D classical statistical mechanical ring polymer theory for consideration as an interpretation of quantum mechanics.

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[8] One could also include relativistic effects through perturbative corrections to the operator of the modified diffusion Eq. (9), mirroring some relativistic corrections often used in the time dependent Schrodinger equation. For the high temperature non-relativistic case, trajectories running from 0 to small β values will contribute negligibly to the electron density so that the system will behave classically as expected. This is shown rigorously in reference [11] appendix C.

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