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Nonlocal approach to energy bands in periodic lattices and emergence of electron mass enhancement

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ABSTRACT

In this study, we analyze energy bands in periodic lattices based on the nonlocal-in-time kinetic energy approach introduced recently by Suykens. We consider the electron dynamics in the periodic potential and construct a nonlocal approach to the weak binding case in three dimensions. A number of features are revealed. In particular, we demonstrate an effective mass enhancement for electrons of around $m^* \approx 167\alpha^{-2}$ Gev/c^2 for typical solids, where α is a real free parameter.

1. Introduction

It is well known that quantum states of light and matter are basically nonlocal, which reflects the fundamental property of wave–-particle duality. Nonlocality is the most fascinating and poorly understood phenomenon in quantum theory, and it generally manifests when measurements (in space or in time) are obtained based on two or more isolated quantum mechanical systems. As a result, physical effects can be technically correlated to some extent, thereby defying any local classical explanation [1], and thus quantum mechanics are considered to be nonlocal. It was argued [1] that an association between Heisenberg's uncertainty principle and nonlocality holds for almost all physical systems and that there is a link between “Einstein's spooky action at a distance” concept and Heisenberg's uncertainty principle. A well-known example of nonlocality is quantum entanglement formulated in terms of the Bell inequalities [2], which was experimentally verified [3,4]. Nonlocality in the broad spectrum occurs in quantum optics [5,6], composite metamaterials [6–9], phononic fluids [10], linear fiber reinforced materials [11], sound propagation in rigid-framed porous media saturated with a viscothermal fluid [12], quantum dynamical pattern formation [13], relativistic oscillators [14], topological insulators [15] or moving media [16] where a macroscopic quantum electrodynamics formulation was recently constructed successfully [17], nanoplasmonics [18], semiconductor plasmonic crystals [19–21], noncrystalline solids [22], plasmonic semiconductor particles [23], multilayered nanocomposites [24], crystals containing a large number of dislocations [25], and other systems.

All of these studies demonstrated that quantum nonlocality is a rich phenomenon that occurs in nature. In general, nonlocal systems are characterized by equations of motion that depend on more than one moment in time, and thus they are characterized by the presence of an infinite sum of higher derivative terms [26,27]. Higher-order derivatives play key roles in several branches of theoretical physics, particularly quantum theories. They arise naturally during the construction of a perturbative approximation to a more fundamental theory. In the present study, we consider nonlocal quantum effects in crystals from a completely different perspective. Our method is based on the concept of Suykens's nonlocal-in-time kinetic energy (SNLTKE), where higher derivative corrections occur only in terms multiplied by a small perturbative nonlocal time parameter [28]. In particular, the equations of motion depend on more than one moment in time, and thus higher derivative terms appear due to the nonlocality in time. Higher-order derivative theories are a major motivating challenge in science. Suykens's approach is motivated by Feynman's tactic, which replaces the square of the velocity $\dot{x}^2$ in the kinetic energy by $\frac{x_{k+1}-x_k}{\varepsilon}\frac{x_k-x_{k-1}}{\varepsilon}$, where $\varepsilon = t_{i+1} - t_i$ and x is the displacement. This is nothing more than shifting backward and forward in time for the body position. However, in Suykens's approach, the $\dot{x}^2$ term is replaced by $\dot{x}\frac{\Delta}{2}$, where $\Delta = \dot{x}(t+\tau) + \dot{x}(t-\tau)$ and τ is a very small parameter called the “nonlocal time parameter.” Obviously, higher derivative corrections occur in terms multiplied by τ after series expansions of Δ given that $x(t+\tau) \approx x(t) + \sum_{k=1}^{n} \frac{\tau^k}{k!}x^{(k)}(t)$ and $x(t-\tau) \approx x(t) + \sum_{k=1}^{n} \frac{(-\tau)^k}{k!}x^{(k)}(t)$. In Suykens's approach, the nonlocal time parameter $\tau << 1$, so it is natural to expand Δ in terms of series at $\tau = 0$. Therefore, the new kinetic energy term is $K_{\tau,n} = \frac{m\dot{x}^2}{2} + \frac{m\dot{x}}{4}\sum_{k=1}^{n} \frac{1+(-1)^k}{k!}\tau^k x^{(k+1)}$ (m is the mass of the body). This straightforward nonlocal-in-time scheme leads to a number of interesting properties at all scales, as discussed in previous studies [29–35]. Clearly, higher-order derivative theories are

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characterized by the presence of an infinite number of higher-order temporal derivatives and they do not disagree with the formalism of quantum theory [36–39]. A well-known example is the Abraham–Lorentz theory, which describes the equation of motion for charged particles considering radiative effects [40]. It should be stressed that τ is generally an unknown variable, and thus care must be taken when interpreting its presence in any dynamical theory.

Based on SNLTKE, an acceleratum operator in quantum mechanics was constructed more recently [41]. This new operator was in fact motivated from Caianiello's maximal acceleration which is an upper limit introduced in his geometrical formulation of quantum mechanics [42–45]. In literature, there exists a large number of arguments supporting the existence of a maximal acceleration at classical and quantum levels [46–52]. In fact, the theory of maximal acceleration was applied in various fields of sciences (see Ref. [53] and references therein) yet to the best of our knowledge, the theory was not applied to material sciences. Based on Caianiello's maximal acceleration $a \leq \frac{2mc^3}{\hbar}$ (($\hbar$, c) being respectively the Planck's constant and the celerity of light), an associated quantum operator $\hat{a} = \frac{\hat{\mathbf{p}}c}{\alpha i m}\nabla$ was constructed in Ref. [41] ($\hat{\mathbf{p}} = -i\hbar\nabla$ is the quantum momentum operator, $i = \sqrt{-1} \in \mathbb{C}$, α is a real parameter and ∇ is the gradient). Moreover, since in SNLTKE, the conserved energy/Hamiltonian for a higher-order Lagrangian $\mathbf{L}_{\tau,n}(x, \dot{x}, \ddot{x}, ..., x^{(n+1)}) = K_{\tau,n} - V$ (V being the potential energy) which is not explicitly depending on time is given by Ref. [28]:

$$\mathbf{H}_{\tau,n} = \sum_{k=0}^{n+1}\sum_{j=0}^{k-1}(-1)^j\left(q^{(k-j)}\frac{d^j}{dt^j}\frac{\partial \mathbf{L}_{\tau,n}}{\partial x^{(k)}}\right) - \mathbf{L}_{\tau,n}, \tag{1}$$

so for $n = 2$ (since $\tau << 1$), the Hamiltonian is given by:

$$\mathbf{H}_{\tau,2} = \frac{1}{2}mv^2 + \frac{1}{2}\tau^2 mvJ - \frac{1}{4}\tau^2 ma^2 + V, \tag{2}$$

where $a = \ddot{x}$ is the acceleration and $J = \dot{a}$ is the jerk which is neglected since the acceleration is maximal. The passage to the quantum limit is obtained after replacing $(x, \mathbf{p}, a, \mathbf{H}_{\tau,2}) \to (\hat{x}, \hat{\mathbf{p}}, \hat{a}, \hat{\mathbf{H}}_{\tau,2})$ and we find that [41]:

$$\hat{\mathbf{H}}_{\tau,2} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4}\tau^2\frac{\hbar^2c^2}{\alpha^2 m}\nabla^4 + V. \tag{3}$$

Equation (3) is the nonlocal Schrödinger operator in the sense of SNLTKE and it is the basic operator used in our treatment of nonlocal quantum mechanics in a period lattice such as crystals. It should be noted that the assumed high-order $n = 2$ is sufficient to obtain the correct band structure in a solid. In fact, for $n > 2$, higher-order terms on τ will occur, i.e., τ^4, τ^6, ..., but their impacts on the theory are very weak. Our proposed method predicts that solutions expanded up to $n = 2$ correspond to physical solutions. In reality, quantum mechanics in crystals can be formulated well using Bloch–Floquet wave theory [54,55], which provides a mathematical technique for analyzing the behavior of systems with a periodic structure. However, nonlocality occurs in lattice systems according to different arguments (see Refs. [56–59] and references therein), but the well-known nonlocal lattices are recognized as “fractional lattice models,” which describe fractional lattice vibrational phenomena as a generalization of crystal lattice dynamics [60], and they allow the description of all types of physical fields in the harmonic approximation. These fields are defined on lattices characterized by a continuum limit governed by irregular power-law nonlocality in the form of fractional derivative kernels. As shown in the following, the nonlocal quantum mechanics for periodic lattices based on SNLTKE lead to a number of interesting features based on the higher-order Schrödinger equation but without passing to the fractional approach, which generally requires advanced and tricky numerical analysis, and this is a challenging task. The remainder of this paper is organized as follows. In Section 2, we apply the SNLTKE approach to the band theory of solids, where we analyze the electron dynamics in the periodic potential. In Section 3, we discuss the nonlocal approach to the weak binding case in three spatial dimensions. Finally, we give our conclusions and future perspectives in Section 4.

2. The nonlocal-in-time kinetic approach to electrons in the periodic potential

We start our analysis by deriving the energy dispersion relations $E\left(\vec{k}\right)$ in materials since the transport properties of solids are connected to $E\left(\vec{k}\right)$ and to the variations in $E\left(\vec{k}\right)$ near the Fermi level ($\vec{k}$ is the wave vector). To obtain the required settings for the transport properties, we first analyze the one-dimensional structure where the periodic potential has periodicity b, as introduced by Bloch and Floquet. In the SNLTKE, the wave function $\psi_k(x) = e^{ikx}u_p(x)$ (Bloch's theorem in one spatial dimension), where $u_p(x)$ is a periodic function of x that satisfies $u_p(x + nb) = u_p(x)$, $\forall\, n$, while it also satisfies the relation $\psi_k(x + nb) = e^{ikx}e^{iknb}u_p(x + nb)$ and it is a solution of the nonlocal Schrödinger equation $\hat{\mathbf{H}}_{\tau,2}\psi_k = E\psi_k$ (E is a constant equal to the total energy of the system). We first derive the matching fundamental properties. By using the equations:

$$\nabla^2\psi_k = -k^2e^{ikx}u_p(x) + 2ike^{ikx}u_p'(x) + e^{ikx}u_p''(x), \tag{4}$$

$$\nabla^4\psi_k = k^4e^{ikx}u_p(x) - 4ik^3e^{ikx}u_p'(x) - 6k^2e^{ikx}u_p^{''}(x) + 4ike^{ikx}u_p^{'''}(x) + e^{ikx}u_p^{(4)}(x), \tag{5}$$

we find that:

$$-\frac{\hbar^2}{2m}(-k^2u_p(x) + 2iku_p'(x) + u_p''(x)) - \frac{\tau^2\hbar^2c^2}{4\alpha^2 m}(k^4u_p(x) - 4ik^3u_p'(x) - 6k^2u_p''(x) + 4iku_p^{'''}(x) + u_p^{(4)}(x)) + V_pu_p(x) = Eu_p(x), \tag{6}$$

where $V_p(x + nb) = V_p(x)$ is the periodic potential. The new Hamiltonian operator is now written as:

$$\hat{\mathbf{H}}_{\tau,2}^{p,k} = -\frac{\hbar^2}{2m}\underbrace{(D^2 + 2ikD - k^2)}_{(D+ik)^2} - \frac{\tau^2\hbar^2c^2}{4\alpha^2 m}\underbrace{(D^4 + 4ikD^3 - 6k^2D^2 - 4ik^3D + k^4)}_{(D+ik)^4} + V_p(x), \tag{7}$$

where $D = \frac{d}{dx}$ and $D^n = \frac{d^n}{dx^n}$, $n = 1,2,3, ...$ Clearly, the nonlocal Schrödinger equation $\hat{\mathbf{H}}_{\tau,2}^{p,k}\psi_k = E\psi_k$ may be written in matrix form as:

$$\sum_n <\phi_m|\hat{\mathbf{H}}_{\tau,2}^{p}(k)|\phi_n> b_n = E\sum_k <\phi_m|\phi_n> b_n, \tag{8}$$

by letting $u_p(x) = \sum_{n=1}^{N} b_n\phi_n(x)$ and where the periodic boundary condition is satisfied. The wave function $\phi_n(x)$ is not obligatory orthogonal. The problem involves fixing k in order to solve the generalized eigenvalue problem (8). Note that if we replace $k \to k + \frac{2s\pi}{b}$ (s is an integer), then we can check that $\psi_{k+2s\pi/b}(x) = e^{ikx}U_p(x)$ where $U_p(x) = u_p(x)e^{\frac{2i\pi sx}{b}}$, and thus $U_p(x)$ and $u_p(x)$ comprise the same set of eigenvalues and they are the same eigenfunctions within a multiplicative constant [61]. Thus, E is a periodic function in k with period $\frac{2\pi}{b}$, which is recognized as the Brillouin zone [62]. Moreover, since $\hat{\mathbf{H}}_{\tau,2}$ is real, then $\psi_k^*(x) = e^{-ikx}U_p^*(x)$, where $U_p^*(x)$ satisfies the conjugate of equation (6). It should be noted that the operator:

$$\hat{\mathbf{H}}_{\tau,2}^{p,k} = -\frac{\mathrm{h}^2}{2m}\mathbb{D}^2 - \frac{\tau^2\mathrm{h}^2c^2}{4\alpha^2 m}\mathbb{D}^4 + V_p(x),$$

where $\mathbb{D} = D + ik$ is the self-adjoint or Hermitian operator since it is easy to check that [63–66]: