Comment on "Quantum-Mechanical Position Operator in Extended Systems"

In a recent publication [1] it is shown how to define a quantity for the position expectation value in systems which satisfy periodic boundary conditions (PBC). The motivation to define such a quantity is related to the recent solution of the long-standing problem of dielectric polarization in crystalline solids [2,3]. For defining the position expectation value $\langle x\rangle$ in crystals with PBC Ref. [1] uses the exponential operator

$$\tau\left(\frac{2\pi}{Ma}\right) = \exp\left(i\,\frac{2\pi}{Ma}\,x\right) \tag{1}$$

instead of the coordinate operator x itself. In Eq. (1) Ma is the length of the one-dimensional crystal with M being a large integer and a is the crystal constant. It is, however, claimed in Ref. [1] that the polarization which is proportional to $\langle x\rangle$ is a manifestation of the Berry phase and is therefore "an observable which cannot be cast as an expectation value of any operator." This is a nontrivial claim which holds for the Berry phase, but it is not necessarily applicable to the geometrical phase in the band structure of solids [4].

The main point of the present Comment is actually the casting of the result for $\langle x\rangle$ in Ref. [1] in the form of an expectation value of a well defined Hermitian operator. Thus, it is easy to show that

$$\begin{aligned}\langle x\rangle &= -\frac{a}{2\pi}\sum_{s=1}^{M-1}\operatorname{Im}\ln\int_0^a \psi_{k_s}(r)\exp\left(-i\,\frac{2\pi}{Ma}\,x\right)\psi_{k_s+1}(x)\,dx \\ &= \frac{a}{2\pi}\sum_k\int_0^a \psi_k^*(q)\sin\left[\frac{2\pi}{Ma}\left(i\,\frac{a}{\partial k} + q\right)\right]\psi_k(q)\,dq\,.\end{aligned} \tag{2}$$

The first line of Eq. (2) is the result of Ref. [1], while the second line is written in the kq representation [5] and it gives $\langle x\rangle$ explicitly as an expectation value of the operator $\sin[(2\pi/Ma)x]$ in the state of the Wannier function of the band [it should be pointed out that in the kq representation $\psi_k(q)$ is the Wannier function of the band and $x = i(\partial/\partial k) + q$]. The sine operator in Eq. (2) is $(1/2i)\{\tau(2\pi/Ma) - \tau[-(2\pi/Ma]\}$ [see Eq. (1)] and leads therefore to shifts of the discrete quasimomentum by $2\pi/Ma$ and $-2\pi/Ma$, respectively. The result in Eq. (2) is very interesting because on one hand (first line) it coincides with the discretization [2,3] of the original geometric phase γ in the band structure of solids [5] (infinite crystal)

$$\gamma = \frac{2\pi}{a}\langle x\rangle = \int_0^a\int_0^{2\pi/a} dq\,dk\,\psi_k^*(q)\left(i\,\frac{\partial}{\partial k} + q\right)\psi_k(q) \tag{3}$$

[in normalization of $\psi_k(q)$ as in Eq. (2)] while, on the other hand (line 2), $\langle x\rangle$ in a finite crystal with PBC assumes the same form as in Eq. (3) but with the operator x replaced by $(Ma/2\pi)\sin[(2\pi/Ma)x]$.

This shows that the open path geometric phase can be given as an expectation value of x in the infinite crystal [Eq. (3)] and as an expectation value of $\sin[(2\pi/Ma)x]$ in either for the discretized k-space mesh [6] or for the finite crystal with PBC [Eq. (2)]. This is a far reaching result which shows that in a crystal with PBC the coordinate operator x is to be replaced by the periodic in x operator $(Ma/2\pi)\sin[(2\pi/Ma)x]$. The latter goes over into x when $M\to\infty$. We also point out that in the case with PBC the operator $\tau(2\pi/Ma)$ in Eq. (1) forms a complete set of commuting operators. It is a special case of the kq representation [5] when the quasicoordinate is defined by the operator $\tau(2\pi/Ma)$ in Eq. (1) while the translation operator $T(Ma)$ defining the quasimomentum is a unit operator because of the PBC.

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