Second report on manuscript
by Esteve-Paredes and Placios

Overall I judge that the authors have done a conscientious job in replying to my comments and making corresponding changes in the manuscript.

I still have reservations about the way my comments 1(b) and 1(d) were answered. (Incidentally, the authors misquoted 1(b) with a cut-and-paste typo; the sentence should have read "First, isn't it true that $\langle n\boldsymbol{k}|\boldsymbol{v}|n'\boldsymbol{k}\rangle_v$ in Eq. (1) contains a $\delta_{\boldsymbol{k}\boldsymbol{k}'}$?".) If we accept from other arguments that $\langle n\boldsymbol{k}|\boldsymbol{v}|n'\boldsymbol{k}'\rangle_v$ is diagonal in $\boldsymbol{k}$ (e.g., using that $\boldsymbol{v}$ is a periodic operator), and in view of the $\omega_{n\boldsymbol{k},n'\boldsymbol{k}}$ prefactor, we only have to evaluate $\langle n\boldsymbol{k}|\boldsymbol{r}|n'\boldsymbol{k}\rangle_v$ for $\boldsymbol{k}=\boldsymbol{k}'$ and $n\neq n'$. Here I adopt the notation that $\tilde{\psi}$ are the wave functions normalized to volume $L=Na$ while $\psi=\sqrt{N}\,\tilde{\psi}$ are normalized to a primitive cell. Then in 1D

$$
\begin{aligned}
\langle n\boldsymbol{k}|\boldsymbol{r}|n'\boldsymbol{k}\rangle_v &= \int_0^{Na} dx\, x\, \tilde{\psi}^*_{n\boldsymbol{k}}(x)\tilde{\psi}_{n'\boldsymbol{k}}(x) \\
&= \frac{1}{N}\int_0^{Na} dx\, x\, \psi^*_{n\boldsymbol{k}}(x)\psi_{n'\boldsymbol{k}}(x) \\
&= \frac{1}{N}\sum_{j=0}^{N-1}\int_{ja}^{(j+1)a} dx\, x\, \psi^*_{n\boldsymbol{k}}(x)\psi_{n'\boldsymbol{k}}(x) \\
&= \frac{1}{N}\sum_{j=0}^{N-1}\int_0^{a} dx\, (x+ja)\, \psi^*_{n\boldsymbol{k}}(x)\psi_{n'\boldsymbol{k}}(x)
\end{aligned}
$$

where I have used that $\psi^*_{n\boldsymbol{k}}(x)\psi_{n'\boldsymbol{k}}(x)$ is periodic under $x\to x+a$. Then

$$
\begin{aligned}
\langle n\boldsymbol{k}|\boldsymbol{r}|n'\boldsymbol{k}\rangle_v = &\Big(\frac{1}{N}\sum_{j=0}^{N-1}\Big)\Big(\int_0^a dx\, x\, \psi^*_{n\boldsymbol{k}}(x)\psi_{n'\boldsymbol{k}}(x)\Big) \\
&+\Big(\frac{a}{N}\sum_{j=0}^{N-1} j\Big)\Big(\int_0^a dx\, \psi^*_{n\boldsymbol{k}}(x)\psi_{n'\boldsymbol{k}}(x)\Big)
\end{aligned}
$$

The second integral vanishes by orthogonality of the wave functions and the first factor in the first term is unity, so

$$
\langle n\boldsymbol{k}|\boldsymbol{r}|n'\boldsymbol{k}\rangle_v = \int_0^a dx\, x\, \psi^*_{n\boldsymbol{k}}(x)\psi_{n'\boldsymbol{k}}(x)
$$

I believe another argument along these lines allows to show that $C_{n\boldsymbol{k},n'\boldsymbol{k}}$ can be similarly written in terms of the boundaries of the primitive cell.

This kind of development is what I had in mind when I wrote "I suspect Eqs. (11-12) can be recast in terms of integrals over a the interior and the boundary of a single primitive cell, with wave functions normalized to the unit cell." I leave it as an option for the authors to discuss this somehow in their revised manuscript.