Exciton-Photon Interaction from the Ground Up

Haixuan Lin

Department of Physics, Fudan University

Jul 11, 2026

Excitons are electron-hole pairs bound by the Coulomb interaction and have been at the center of solid-state research for decades. They are essential for opto-electronic and quantum technologies and are actively investigated in these years.

1 Derivation For Exciton-Phonon interaction from the Ground Up

- Photon-Induced Kohn–Sham Scattering
- Exciton Hamiltonian under the Tamm–Dancoff Approximation
- Nondiagonal Terms in Exciton-Phonon Interaction

Derivation For Exciton-Phonon interaction from the Ground Up

Summary

1 Derivation For Exciton-Phonon interaction from the Ground Up

- Photon-Induced Kohn–Sham Scattering
- Exciton Hamiltonian under the Tamm–Dancoff Approximation
- Nondiagonal Terms in Exciton-Phonon Interaction

A Brief Review to DFT

The core idea in Density Functional Theory (DFT) is construct a strict correspondence between interacting many-body system and system without interaction with effective single-particle potential.

In fact, we are only concerned with the final electron dentity $n\left(\mathbf{r}\right)$ in our calculation, thus we can postulate a potential $V_{\mathbf{KS}}\left[n\left(\mathbf{r}'\right)\right]\left(\mathbf{r}\right)$ (KS means Kohn and Sham) as a variational funcional of $n\left(\mathbf{r}'\right)$ and write down a single-particle Schrödinger equation:

$$\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2+V_{\mathrm{KS}}\left[n\left(\mathbf{r}'\right)\right]\left(\mathbf{r}\right)\right)\phi_i\left(\mathbf{r}\right)=\varepsilon_i\phi_i\left(\mathbf{r}\right), \tag{1}$$

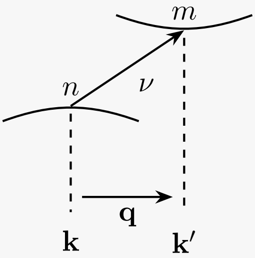
where $n\left(\mathbf{r}\right)=\sum_i\left|\phi_i\left(\mathbf{r}\right)\right|^2$.

Kohn and Sham had used variational method and derived

$$V_{\mathrm{KS}}\left[n\left(\mathbf{r}'\right)\right](\mathbf{r}) = \underbrace{V_0(\mathbf{r})}_{\text{ion potential}} + \underbrace{e^2\int\frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\mathrm{d}\mathbf{r}'}_{\text{Hatree potential}} + \underbrace{\frac{\delta E_{\mathrm{xc}}[n(\mathbf{r}')]}{\delta n(\mathbf{r})}}_{\text{exchange potential}}. \tag{2}$$

And in feasible calculation, V_0 are usually substituted by pseudo potential.

Electron-Phonon Interaction



Let's take lattice distortion into account when derive Kohn–Sham potential. To first order in Fermi's golden rule, we deem phonon as perturbation, then

$$g_{mn,\nu}(\mathbf{k},\mathbf{q}) = \langle m\mathbf{k}+\mathbf{q}|\,\Delta V_{\nu\mathbf{q}}\,|n\mathbf{k}\rangle\,, \qquad (3)$$

where $g_{mn,\nu}(\mathbf{k},\mathbf{q})$ is the phonon-induced scattering matrix element of electron, $\Delta V_{\nu\mathbf{q}}$ is the perturbative potenial.

$$\hat{H}_{\text{e-ph}} = \sum_{mn\nu\mathbf{k}\mathbf{q}} g_{mn,\nu}(\mathbf{k},\mathbf{q})\,\hat{c}^{\dagger}_{m\mathbf{k}+\mathbf{q}}\hat{c}_{n\mathbf{k}}\left(\hat{b}_{\nu\mathbf{q}} + \hat{b}^{\dagger}_{\nu-\mathbf{q}}\right) \qquad (4)$$

Summary

A Brief Review to Lippmann–Schwinger–Born Series

The Lippmann–Schwinger–Born Series is known for its equivalence to the Schrödinger equation $\left(E - \hat{H}_0\right) |\psi\rangle = \hat{V} |\psi\rangle$ but plentiful physical picture.

Write down the formal solution with general solution of associated homogeneous equation:

$$|\psi\rangle = \frac{1}{E - \hat{H}_0 \pm \mathrm{i}0^+} \hat{V} |\psi\rangle + |\mathbf{k}\rangle .$$

This is actually an equivalent integral equation, which is suitable for iteration:

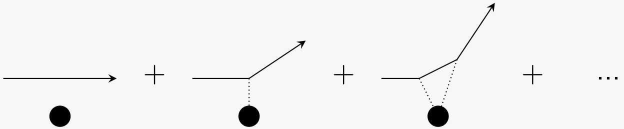
$$|\psi_{n+1}\rangle = \frac{1}{E - \hat{H}_0 \pm \mathrm{i}0^+} \hat{V} |\psi_n\rangle + |\mathbf{k}\rangle ,$$

where $|\psi_0\rangle = |\mathbf{k}\rangle$.

After iteration scheme, then

$$|\psi\rangle = \sum_{n=0}^{\infty} \left(\frac{1}{E - \hat{H}_0 \pm \mathrm{i}0^+} \hat{V} \right)^n |\mathbf{k}\rangle. \tag{5}$$

This form depicts that the scattering process is essentially a superposition of elementary interactions of different orders.



No Scattering | Single Scattering | Double Scattering | Multiple Scattering

Exciton Hamiltonian

In rigorous mechanics, the state of one exciton is permitted to contain "imaginary components", which are contributed by the process that annihilates an exciton-hole pair. In Tamm–Dancoff approximation, we only consider the positive process:

$$|S_n(\mathbf{Q})\rangle = \sum_{vc} A_{vc}^{S_n(\mathbf{Q})} |vc\rangle, \tag{6}$$

where $|vc\rangle = \hat{c}_c^\dagger \hat{c}_v |0_\mathrm{F}\rangle$. Substitute it into the Schrödinger equation of exciton:

$$\sum_{v'c'} H_{vc,v'c'} A_{v'c'}^{S_n(\mathbf{Q})} = E^{S_n(\mathbf{Q})} A_{vc}^{S_n(\mathbf{Q})}. \tag{7}$$

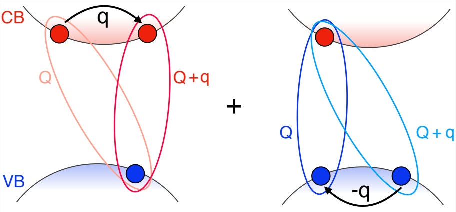
And in first order perturbation accuracy,

$$\tilde{H} = \sum_{n\mathbf{Q}} E^{S_n(\mathbf{Q})} \hat{a}^\dagger_{S_n(\mathbf{Q})} \hat{a}_{S_n(\mathbf{Q})} + \sum_{\nu\mathbf{q}} \hbar\omega_{\nu\mathbf{q}} \hat{b}^\dagger_{\nu\mathbf{q}} \hat{b}_{\nu\mathbf{q}} + \sum_{nm\nu,\mathbf{Q}\mathbf{q}} \mathcal{G}_{nm\nu}(\mathbf{Q},\mathbf{q}) \hat{a}^\dagger_{S_m(\mathbf{Q}+\mathbf{q})} \hat{a}_{S_n(\mathbf{Q})} (\hat{b}_{\nu\mathbf{q}} + \hat{b}^\dagger_{\nu-\mathbf{q}}), \tag{8}$$

where $\mathcal{G}_{nm\nu}(\mathbf{Q},\mathbf{q})$ depicts the interaction between excitons and phonons.

Summary

$$
\begin{aligned}
&\mathcal{G}_{nm\nu}(\mathbf{Q},\mathbf{q}) \\
&= \sum_{\mathbf{k}} \Bigg[\sum_{vcc'} A^{S_m(\mathbf{Q}+\mathbf{q})*}_{v\mathbf{k},c(\mathbf{k}+\mathbf{Q}+\mathbf{q})} A^{S_n(\mathbf{Q})}_{v\mathbf{k},c'(\mathbf{k}+\mathbf{Q})} g_{c'c\nu}(\mathbf{k}+\mathbf{Q},\mathbf{q}) \\
&\quad - \sum_{cvv'} A^{S_m(\mathbf{Q}+\mathbf{q})*}_{v(\mathbf{k}-\mathbf{q}),c(\mathbf{k}+\mathbf{Q})} A^{S_n(\mathbf{Q})}_{v'\mathbf{k},c(\mathbf{k}+\mathbf{Q})} g_{vv'\nu}(\mathbf{k}-\mathbf{q},\mathbf{q}) \Bigg]
\end{aligned} \tag{9}
$$



References

[1] H.-Y. Chen, D. Sangalli, and M. Bernardi, "Exciton-phonon interaction and relaxation times from first principles," *Physical Review Letters*, vol. 125, no. 10, p. 107 401, Aug. 2020. DOI: 10.1103/PhysRevLett.125.107401. https://doi.org/10.1103/PhysRevLett.125.107401.

The End