Polaron physics: some recent developments

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Outline of the talk

- Introduction to coupled electron-phonon systems; the polaron concept

  [VMS and M. Vanevic, PRB 78, 214301 (2008)]
  [D. J. J. Marchand et al., arXiv:1010.3207 (2010)]
  [VMS, N. Vukmirovic, and C. Bruder, PRB 82, 165410 (2010)]
  [N. Vukmirovic, VMS, and M. Vanevic, PRB 81, 041408(R) (2010)]

Conclusions and Outlook

VMS

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Non-analyticities in a polaron model and recent corroboration

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- Further implications of strongly momentum-dependent electron-phonon coupling
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- Conclusions and Outlook
**Polaron: generalities**

**Polaron concept:**
L. D. Landau (1933), polar semiconductors (alkali-halides)

**Polarons also found in:**
transition-metal oxides, glasses, organic semiconductors, undoped cuprates, etc.

**main feature:**
low-mobility ($\mu < 1 \text{ cm}^2/\text{Vs}$), increasing with temperature!

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**D. Emin, 1982:** “...Small polaron is an extra electron or a hole severely localized within a potential well that it creates by displacing the atoms that surround it...”
Central tenet: Polaron models show smooth crossovers between weak- and strong-coupling regimes!

No sharp transitions – is this always true?
Generic coupled electron-phonon model

\[
\hat{H} = \hat{H}_e + \hat{H}_{ph} + \hat{H}_{e-ph}
\]

\[
\hat{H}_e = -t \sum_i (\hat{a}^\dagger_{i+1} \hat{a}_i + \text{h.c.})
\]

\[
\hat{H}_{ph} = \sum_q \omega(q) \hat{b}^\dagger_q \hat{b}_q
\]

translational invariance: \([\hat{H}, \hat{K}] = 0\) regardless of the form of \(\hat{H}_{e-ph}\)

\[
\hat{K} = \sum_k k \hat{a}^\dagger_k \hat{a}_k + \sum_q q \hat{b}^\dagger_q \hat{b}_q
\]

total crystal momentum operator

\[
\hat{K} |\psi_\kappa\rangle = \kappa |\psi_\kappa\rangle
\]

\[
\hat{H} |\psi_\kappa\rangle = E_\kappa |\psi_\kappa\rangle
\]
Quasiparticle weight and effective mass

quasiparticle weight (residue) at momentum $k$ in band $n$:

$$Z_n(k) \equiv |\langle \Psi_{nk} | \psi_{nk} \rangle|^2 \quad (0 < Z_n(k) < 1)$$

ratio of the effective ($m_{\text{eff}}$) and bare band ($m_{e}^*$) electron masses

$$\frac{m_{\text{eff}}}{m_{e}^*} = \lim_{k \to 0} \frac{\varepsilon(k) - \varepsilon(0)}{E(k) - E(0)}$$

$$\varepsilon(k) = -2t \cos k \Rightarrow m_{e}^* \equiv (2t)^{-1}$$

renormalized dispersion: $E(k) = \varepsilon(k) + \text{Re} \Sigma[k, E(k)]$

$$\left(\frac{m_{\text{eff}}}{m_{e}^*}\right)_\alpha = \frac{Z^{-1}(k = 0)}{1 + \left. \frac{\partial}{\partial \varepsilon(k_\alpha)} \text{Re} \Sigma(k_\alpha, \omega) \right|_{k_\alpha=0, \omega=E(0)}}$$

$k_\alpha \equiv k \cdot \hat{e}_\alpha$
Molecular-crystal model

local (Holstein-type) coupling

\[ \hat{u}_i \equiv \frac{1}{\sqrt{2m\omega}} (\hat{b}^\dagger_i + \hat{b}_i) \]

dispersionless phonons:

\[ \hat{H}_{ph} = \omega \sum_i \hat{b}^\dagger_i \hat{b}_i \]

displacement at site \( i \):

\[ \epsilon \rightarrow \epsilon + \alpha_H u_i \]

non-local (Peierls-type) coupling

\[ t \rightarrow t + \alpha_P (u_{i+1} - u_i) \]

central tenet of the theory:

SMOOTH CROSOVERS

NO SHARP TRANSITION!
Common types of short-range e-ph coupling

**Holstein-type (local) coupling:**

\[
\hat{H}_g = g\omega \sum_i \hat{a}_i \hat{a}_i (\hat{b}_i^\dagger + \hat{b}_i)
\]

**Peierls-type (nonlocal) coupling:**

\[
\hat{H}_\phi = \phi \omega \sum_i (\hat{a}_{i+1}^\dagger \hat{a}_i + \text{h.c.}) (\hat{b}_{i+1}^\dagger + \hat{b}_{i+1} - \hat{b}_i^\dagger - \hat{b}_i)
\]

electron current operator: \( \hat{J} = -ie t \sum_j (\hat{a}_{j+1}^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{a}_{j+1}) \)

in the presence of Peierls’ coupling \( \Rightarrow \) “phonon-assisted” current:

\[
\hat{J} = -ie \sum_j \left[ t + \phi \omega (\hat{b}_{j+1}^\dagger + \hat{b}_{j+1} - \hat{b}_j^\dagger - \hat{b}_j) \right] (\hat{a}_{j+1}^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{a}_{j+1})
\]
Peierls-type electron-phonon coupling

Sir Rudolf Peierls (1907-1995)

π-electron hopping integral is dynamically bondlength-dependent:

\[ t \to t(\Delta u_{cc}) \approx t + \alpha \Delta u_{cc} \]

also known as

- Su-Schrieffer-Heeger (SSH)
- Barišić-Labbé-Friedel (BLF)

coupling
Examples of systems with Peierls-type coupling (I)

organic molecular crystals, e.g., polyacenes

Examples of systems with Peierls-type coupling (II)

graphene-based systems, e.g., graphene antidot lattices

See, e.g., VMS, N. Vukmirović, and C. Bruder, PRB 82, 165410 (2010)
Momentum dependence of electron-phonon coupling

\[
\hat{H}_{e-ph} = N^{-1/2} \sum_{k,q} \gamma(k, q) \hat{a}^\dagger_{k+q} \hat{a}_k (\hat{b}^\dagger_{-q} + \hat{b}_q)
\]

1. momentum-independent couplings

Holstein-type (local) coupling: \( \gamma_H(k, q) = g\omega = \text{const.} \)

2. momentum-dependent couplings

- Coupling to the “breathing” modes in cuprates:
  \[
  \gamma_B(k, q) = \gamma_B(q) \propto \sqrt{\sin^2(q_x/2) + \sin^2(q_y/2)}
  \]

- SSH coupling in a one-dimensional or square lattice:
  \[
  \gamma_{SSH}(k, q) \propto \sin(k \cdot a) - \sin[(k + q) \cdot a]
  \]
  \[
  \gamma_{SSH}(k = 0, q) \propto |q| \rightarrow 0 \quad (q \rightarrow 0)
  \]
Two important dimensionless parameters

1. **the adiabaticity ratio:** $\omega / t$

   \[ \text{adiabatic } \omega / t < 1; \text{ non-adiabatic } \omega / t > 1 \]

2. **the (effective) coupling strength:**

   \[
   \lambda = \frac{\langle |\gamma(k, q)|^2 \rangle_{BZ}}{2t\omega} \quad \langle \ldots \rangle_{BZ} \equiv \Omega_{BZ}^{-2} \int_{-\pi/a}^{\pi/a} dk \int_{-\pi/a}^{\pi/a} dq [\ldots]
   \]

   Holstein-type coupling: $\lambda = \frac{g^2 \omega}{2t}$

   Peierls-type coupling: $\lambda = \frac{2\phi^2 \omega}{t}$
Entanglement measures

bipartite system: \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \)

the reduced density matrix of system A: \( \hat{\rho}_A = \text{Tr}_B \hat{\rho} \)

the von Neumann entropy \( S = -\text{Tr}_A (\hat{\rho}_A \ln \hat{\rho}_A) \)

linear entropy (tangle) \( S_L = 1 - \text{Tr}_A (\hat{\rho}_A^2) \)

Our case: \( A \rightarrow e, \quad B \rightarrow \text{ph} \)

OPEN QUESTION:

Are there any nonanalyticities in the e-ph entanglement entropies as a function of coupling strength?
STATE OF THE ART

- **Quantum spin models**: Entanglement measures do not necessarily show nonanalytic behavior at the transition point!
  
  \[ \text{A. Osterloh et al., Nature 416, 608 (2002);} \]
  \[ \text{T. J. Osborne & M. A. Nielsen, PRA 66, 032110 (2002).} \]

- **Quantum-dissipative models**: nonanalytic behavior away from the actual quantum phase transitions!
  
  \[ \text{T. Stauber & F. Guinea, PRA 73, 042110 (2006);} \]
  \[ \text{K. Le Hur, Ann. Phys. 323, 2208 (2008).} \]
Quantum-entanglement aspects of polaron systems

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We describe quantum entanglement inherent to the polaron ground states of coupled electron-phonon (or, more generally, particle-phonon) systems based on a model comprising both local (Holstein-type) and nonlocal (Peierls-type) couplings. We study this model using a variational method supplemented by the exact numerical diagonalization on a system of finite size. By way of subsequent numerical diagonalization of the reduced density matrix, we determine the particle-phonon entanglement as given by the von Neumann and linear entropies. Our results are strongly indicative of the intimate relationship between the particle localization/delocalization and the particle-phonon entanglement. In particular, we find a compelling evidence for the existence of a nonanalyticity in the entanglement entropies with respect to the Peierls-coupling strength. The occurrence of such nonanalyticity—not accompanied by an actual quantum phase transition—reinforces analogous conclusion drawn in several recent studies of entanglement in the realm of quantum-dissipative systems. In addition, we demonstrate that the entanglement entropies saturate inside the self-trapped region where the small-polaron states are nearly maximally mixed.

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Variational Ansatz: inner workings

Bloch wave-functions (eigenstates of the total crystal momentum):

\[ |\psi_\kappa\rangle = N^{-1/2} \sum_n e^{i\kappa n} |\psi_\kappa(n)\rangle \]

Entangled “form-factor” (20 variational parameters):

\[ |\psi_\kappa(n)\rangle = \sum_m \Phi_\kappa(m) e^{i\kappa m} \hat{a}_{n+m}^\dagger |0\rangle \otimes \prod_q \hat{D} \left( - \frac{e^{-i\kappa n} w_\kappa^*(q)}{\sqrt{N}} \right) |0\rangle_{ph} \]

[ Glauber’s displacement operator \( \hat{D}(\alpha_q) |0\rangle_{ph} = |\alpha_q\rangle_{ph} \) ]

\[ \hat{\rho}_{e-ph} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} \implies \hat{\rho}_e = \text{Tr}_{ph}[\hat{\rho}_{e-ph}] \implies S = -\text{Tr}_e(\hat{\rho}_e \ln \hat{\rho}_e) \]
Results from variational method for $t/\omega = 1.0$

Energy is a continuous function of $g$ and $\phi$, while $S$ and $S_L$ are smooth only with respect to $g$!
Exact diagonalization approach

\[ \mathcal{H} = \mathcal{H}_e \otimes \mathcal{H}_{\text{ph}} \]

to states with the total of at most \( M \) phonons

\[ |\Psi\rangle = \sum_{n,m} C_{n,m} |n\rangle_e \otimes |m\rangle_{\text{ph}} \]

Dimension of the truncated Hilbert space:

- \( N = 6 \) sites, \( M = 8 \) phonons \( \rightarrow \) \( D = 7722 \)
- \( M = 9 \) phonons \( \rightarrow \) \( D = 12012 \)
- \( M = 10 \) phonons \( \rightarrow \) \( D = 18018 \)
Non-analyticities with respect to Peierls-type coupling

Entanglement entropies show non-analytic behavior with respect to $\phi$!

Saturation for strong coupling
D. J. J. Marchand et al., arXiv:1010.3207
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NO “universality”: non-analytic behavior does not show up for any $k$- and $q$-dependent coupling!

**Example**: Edwards’ particle-boson coupling model

[A. Alvermann, D. M. Edwards, and H. Fehske, PRL 98, 056602 (2007)]

\[
\hat{H}_{p-b} = -t_b \sum_{\langle i,j \rangle} \hat{a}_j^\dagger \hat{a}_i \left[ \hat{b}_i^\dagger + \hat{b}_j \right]
\]

\[
\Rightarrow \quad \hat{H}_{p-b} = -\frac{2t_b}{\sqrt{N}} \sum_{k,q} \hat{a}_{k+q}^\dagger \hat{a}_k \left[ \cos(k + q) \hat{b}_{-q}^\dagger + \cos(q) \hat{b}_q \right]
\]

does not show a non-analytic behavior!
Another very recent work:


quantal SSH model in 1D, 2D, and 3D with acoustic, rather than optical, phonons

⇒ does not show any non-analytic behavior!

in this model, mass renormalization can be rather different than $Z^{-1}(k = 0)$!
Strongly momentum-dependent electron-phonon coupling

important quantity:

$$|\gamma_{cc}^\lambda(k = 0, q)|$$

strongest coupling to the highest-energy optical phonon!

For this branch

$$|\gamma_{cc}^\lambda(k = 0, q)|$$

largest at $q = 0$!

⇒ expect large mass enhancement!
Conclusions and Outlook

- SSH model (Peierls’ type coupling) shows a non-analytic behavior at a critical coupling strength
- Study the quantal SSH model in higher dimensions
- Experimental implications (ARPES, transport)