Rotation of quantum impurities in the presence of a many-body environment

PRL **114**, 203001 (2015)

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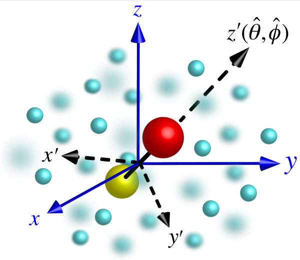
Abstract: We develop a microscopic theory describing a quantum impurity whose rotational degree of freedom is coupled to a many-particle bath. We approach the problem by introducing the concept of an "angulon" – a quantum rotor dressed by a quantum field – and reveal its quasiparticle properties using a combination of variational and diagrammatic techniques. Our theory predicts renormalisation of the impurity rotational structure, such as observed in experiments with molecules in superfluid helium droplets, in terms of a rotational Lamb shift induced by the many-particle environment. Furthermore, we discover a rich many-body-induced fine structure, emerging in rotational spectra due to a redistribution of angular momentum within the quantum many-body system.

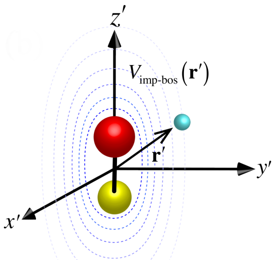
Journal Club, 26/05/2015

Outline

Setup (I)/(II)

- A rotating impurity in a many-body system (MBS)
- MBS is interacting bosons, treated in Bogoliubov approximation
- Impurity is not moving besides its rotation
- Example: Impurity is a linear rotor
- Impurity-MBS coupling depends on orientation





Setup (II)/(II)

Total Hamiltonian:

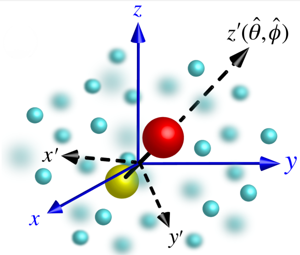
$H = H_{\text{bos}} + H_{\text{imp}} + H_{\text{imp-bos}}$

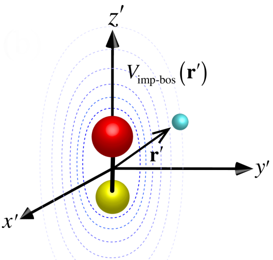
- Impurity: $H_{\text{imp}} = B\hat{\mathbf{J}}^2$
- Bosons:

$$H_{\text{bos}} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} + g_{\text{bb}} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \hat{a}^\dagger_{\mathbf{k}'-\mathbf{q}} \hat{a}^\dagger_{\mathbf{k}+\mathbf{q}} \hat{a}_{\mathbf{k}'} \hat{a}_{\mathbf{k}}$$

- Impurity-boson coupling:

$H_{\text{imp-bos}} =$
$\sum_{\mathbf{k},\mathbf{q}} V_{\text{imp-bos}}(\mathbf{q}, \hat{\theta}, \hat{\phi}) \hat{a}^\dagger_{\mathbf{k}-\mathbf{q}} \hat{a}_{\mathbf{k}}$





Strategy

1. Treat (many-body) bath bosons with Bogoliubov theory and write their Hamiltonian in terms of phonons.
2. Express the impurity-boson coupling and the total Hamiltonian with a "rotation-friendly" basis.
3. Solution of the effective theory with an ansatz and a variational treatment equivalent to a diagrammatic approach that also allows for the computation of the excitations and the spectral function.

Effective Bogoliubov Hamiltonian

- Bogoliubov transform → "phonons" with dispersion ω_k.
  $H = B\mathbf{J}^2 + \sum_{\mathbf{k}} \omega_k \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \sqrt{n} \sum_{\mathbf{k}} V_{\text{imp-bos}}(\mathbf{k}, \hat{\theta}, \hat{\phi}) \sqrt{\frac{\epsilon_{\mathbf{k}}}{\omega_{\mathbf{k}}}} (\hat{b}_{\mathbf{k}} + \hat{b}^\dagger_{-\mathbf{k}})$
- Dropped $\sim \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}}$, which is suppressed by $1/\sqrt{n}$
- Dropped mean-field shift $\sim V(\mathbf{0})n$
- Note: $\sum_{\mathbf{k}} \equiv \int d^3k/(2\pi)^3$.

Hamiltonian in spherical basis (I)/(II)

- Express creation/annihilation operators in spherical harmonics:
  $\hat{b}^\dagger_{\mathbf{k}} = \frac{(2\pi)^{3/2}}{k} \sum_{\lambda\mu} \hat{b}^\dagger_{k\lambda\mu} \; i^{-\lambda} \; Y_{\lambda\mu}(\Theta_k, \Phi_k)$
  $\hat{b}^\dagger_{k\lambda\mu} = \frac{k}{(2\pi)^{3/2}} \int d\Phi_k d\Theta_k \; \sin\Theta_k \; \hat{b}^\dagger_{\mathbf{k}} \; i^{\lambda} \; Y^*_{\lambda\mu}(\Theta_k, \Phi_k)$
- $\lambda \equiv$the angular momentum (AM) of the bosonic excitation
  $\mu \equiv$ AM projection onto the laboratory-frame z-axis.
- Commutation relations:
  $[\hat{b}_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}] = (2\pi)^3 \delta^{(3)}(\mathbf{k} - \mathbf{k}')$ and
  $[\hat{b}_{k\lambda\mu}, \hat{b}^\dagger_{k'\lambda'\mu'}] = \delta(k - k')\delta_{\lambda\lambda'}\delta_{\mu\mu'}$

Hamiltonian in spherical basis (II)/(II)

- Transformed Hamiltonian:

$$H = B\mathbf{J}^2 + \sum_{k\lambda\mu} \omega_k \hat{b}^\dagger_{k\lambda\mu} \hat{b}_{k\lambda\mu} + \sum_{k\lambda\mu} U_\lambda(k) \left[Y^*_{\lambda\mu}(\hat{\theta},\hat{\phi}) \hat{b}^\dagger_{k\lambda\mu} + Y_{\lambda\mu}(\hat{\theta},\hat{\phi}) \hat{b}_{k\lambda\mu} \right]$$

- Note: $\sum_k \equiv \int dk$
- $$U_\lambda(k) = \tilde{V}_\lambda(k) k \sqrt{n\epsilon_{\mathbf{k}}/\omega_{\mathbf{k}}} = u_\lambda \left[\frac{8nk^2\epsilon_k}{\omega_k(2\lambda+1)} \right]^{1/2} \int dr r^2 f_\lambda(r) j_\lambda(kr).$$
- Note: Only $\lambda = 0, 1$ are considered.

Variational/diagrammatic treatment (I)/(III)

- Ansatz:

$$|\psi\rangle = Z_{LM}^{1/2}\,|0\rangle\,|LM\rangle + \sum_{\substack{k\lambda\mu\\ jm}} \beta_{k\lambda j}^{LM}\, C_{jm,\lambda\mu}^{LM}\, \hat{b}^{\dagger}_{k\lambda\mu}\,|0\rangle\,|jm\rangle$$

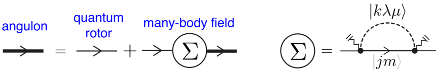
- $|0\rangle \equiv$ vacuum of bath excitations; the angulon quasiparticle weight Z is given by normalisation $Z_{LM} \equiv 1 - \sum_{k\lambda j} |\beta_{k\lambda j}^{LM}|^2$
- Note: $|\psi\rangle$ is an eigenstate of the total AM, $\hat{\mathbf{L}}^2|\psi\rangle = L(L+1)|\psi\rangle$, and its projection on the laboratory z-axis, $\hat{L}_z|\psi\rangle = M|\psi\rangle$
- $C_{jm,\lambda\mu}^{LM}$ is a Clebsch-Gordan coefficient.
- M is irrelevant in the absence of external fields.

Variational/diagrammatic treatment (II)/(III)

- Minimization of $E = \langle\psi| H |\psi\rangle / \langle\psi|\psi\rangle$, where $\langle\psi|\psi\rangle = 1$ yields E_L from $\left[G_L^{\text{ang}}(E_L)\right]^{-1} = 0$.
- Self-consistent equation: $\left[G_L^{\text{ang}}(E)\right]^{-1} = [G_L^0(E)]^{-1} - \Sigma_L(E)$, where $[G_L^0(E)]^{-1} = -E + BL(L+1)$
- Self energy:

$$\Sigma_L(E) = \sum_{k\lambda j} \frac{2\lambda+1}{4\pi} \frac{U_\lambda(k)^2 \left[C_{L0,\lambda 0}^{j0}\right]^2}{Bj(j+1) - E + \omega_k}.$$

- Note: equivalent to Dyson equation $G^{\text{ang}} = G^0 + G^0 \Sigma G^{\text{ang}}$

with diagram: 

Variational/diagrammatic treatment (III)/(III)

- Equivalence to diagrammatic treatment computation of spectrum from retarded Green's function:

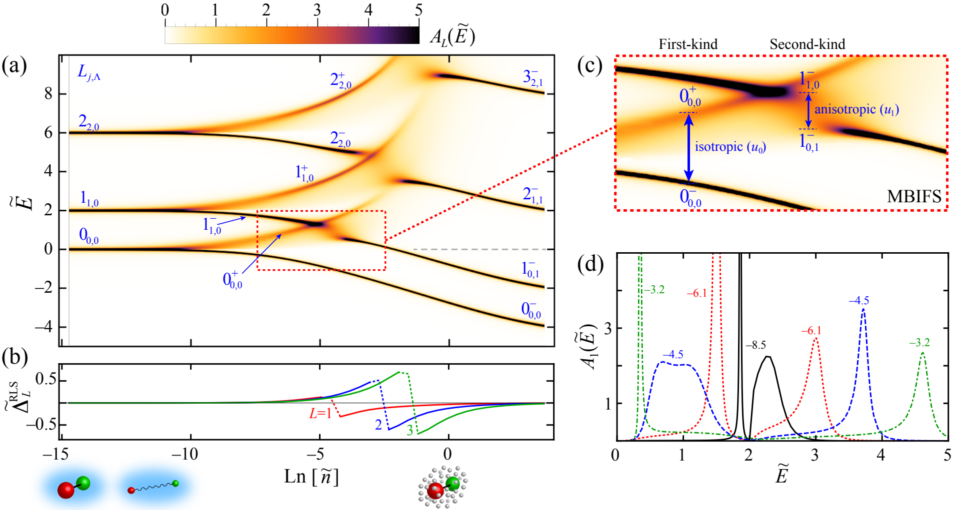
$$G_L^{\text{ret}}(E) = G_L^{\text{ang}}(E + i0^+)$$

- Imaginary part of self-energy of G_L^{red}:

$$\text{Im}\Sigma_L^{\text{ret}}(E) = \sum_{\lambda j k_0} \theta(E - Bj(j+1)) \left[C_{L0,\lambda 0}^{j0} \right]^2 \times \frac{2\lambda+1}{4} U_\lambda(k_0)^2 |(\partial\omega_k/\partial k)_{k=k_0}|^{-1}$$

- k_0 gives the roots of $E - \omega_k + Bj(j+1) = 0$
- Spectral function $\mathcal{A}_L(E) = \text{Im}[G_L^{\text{ret}}(E)]$

Spectral function & rotational Lamb shift



$$\tilde{\Delta}_L^{\mathrm{RLS}} = (E_L - E_0)/B - L(L+1)$$

- Effective theory/Hamiltonian to deal with rotating impurities
- Redistribution of AM between impurity and bath
- Rich physics of the angulon quasiparticle
  - many-body induced fine structure of 1st kind $L_{L,0} \to \{L^-_{L,0}, L^+_{L,0}\}$ and 2nd kind $L^-_{L,0} \to L^-_{L-1,1}$
  - rotational Lamb shift

Open questions: What if the many-body bath cannot be accurately treated with the Bogoliubov approach and/or is not bosonic? What about superposition states of the rotating impurity? What about the contributions of higher harmonics $\lambda > 1$?

Impurity-boson coupling in a spherical basis (I)

- $V_{\text{imp-bos}}(\mathbf{q},\hat{\theta},\hat{\phi}) = \mathcal{F}[R(\hat{\theta},\hat{\phi})V_{\text{imp-bos}}(\mathbf{r}')]$; here, R is a rotation and $\mathcal{F}$ the Fourier transform.
- Expand with spherical harmonics: $\sum_\lambda u_\lambda f_\lambda(r')Y_{\lambda 0}(\Theta',\Phi')$
- Use Wigner rotation matrices $D^\lambda_{\mu\nu}$ to express Ys: $Y_{\lambda 0}(\Theta',\Phi') = \sum_\mu D^{\lambda *}_{\mu 0}(\hat{\phi},\hat{\theta},\hat{\gamma})Y_{\lambda\mu}(\Theta,\Phi)$, here $(\hat{\phi},\hat{\theta},\hat{\gamma})$ are Euler angles.
- For a linear rotor $\hat{\gamma}=0$. Using $D^{\lambda *}_{\mu 0}(\hat{\phi},\hat{\theta},0) = \sqrt{\frac{4\pi}{2\lambda+1}}Y_{\lambda\mu}(\hat{\theta},\hat{\phi})$, one gets: $V_{\text{imp-bos}}(\mathbf{r},\hat{\theta},\hat{\phi}) = \sum_{\lambda\mu}\sqrt{\frac{4\pi}{2\lambda+1}}u_\lambda f_\lambda(r)Y_{\lambda\mu}(\Theta,\Phi)Y_{\lambda\mu}(\hat{\theta},\hat{\phi})$.

Impurity-boson coupling in a spherical basis (II)

- To obtain $V_{\text{imp-bos}}(\mathbf{k},\hat{\theta},\hat{\phi})$, compute Fourier transform of $V_{\text{imp-bos}}(\mathbf{r},\hat{\theta},\hat{\phi}) = \sum_{\lambda\mu} \sqrt{\frac{4\pi}{2\lambda+1}} u_\lambda f_\lambda(r) Y_{\lambda\mu}(\Theta,\Phi) Y_{\lambda\mu}(\hat{\theta},\hat{\phi})$.
- In the Fourier transform, expand $e^{-i\mathbf{kr}}$ in terms of spherical harmonics:
  $V_{\text{imp-bos}}(\mathbf{k},\hat{\theta},\hat{\phi}) \equiv \int d^3\mathbf{r}\ V_{\text{imp-bos}}(\mathbf{r},\hat{\theta},\hat{\phi})\ e^{-i\mathbf{kr}}$
  $= \sum_{\lambda\mu} (2\pi)^{3/2} i^{-\lambda} \tilde{V}_\lambda(k) Y_{\lambda\mu}(\Theta_k,\Phi_k) Y_{\lambda\mu}(\hat{\theta},\hat{\phi})$
- Note: $\mathbf{k} \equiv (k,\Theta_k,\Phi_k)$ is the momentum vector in the laboratory frame.
- $\tilde{V}_\lambda(k) = u_\lambda 2^{3/2}/\sqrt{2\lambda+1} \int_0^\infty dr\, r^2 f_\lambda(r) j_\lambda(kr)$, with $j_\lambda(kr)$ the spherical Bessel function.