Extending Feynman's variational path integral approach: Application to the Bose polaron problem.

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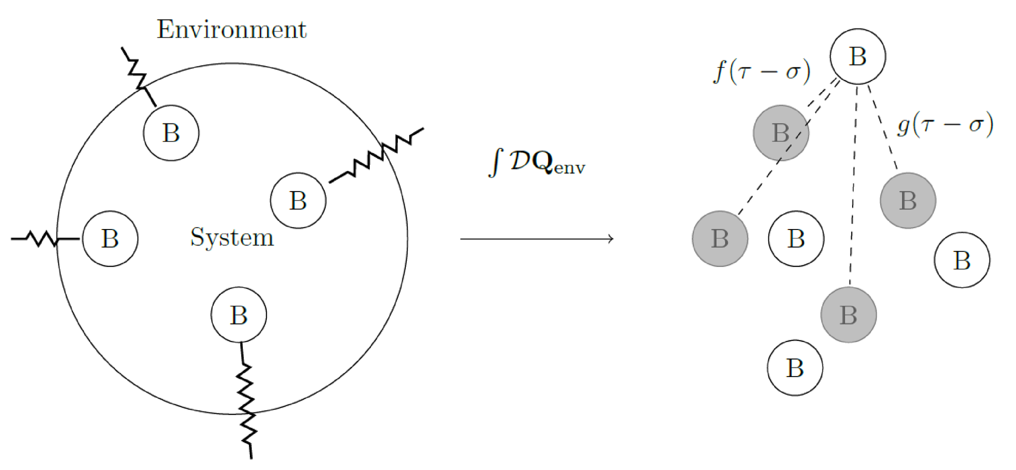
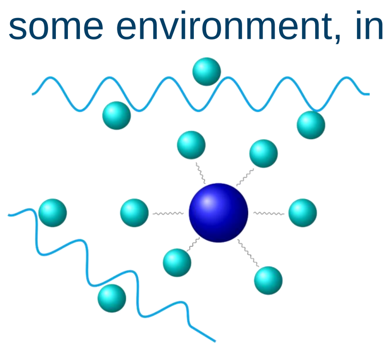
Memory in the polaron problem



When the environment of an embedded system is integrated out in the path-integral description, the remaining system is described as having obtained an effective memory where the particles interact with their positions at previous times through retarded interactions.

This point of view has proven to be very useful for variational approaches in the literature, where usually specific choices for model environments are proposed [1,2,3]. One famous example is the polaron problem where an impurity is interacting with the excitations of some environment, in many cases described through the Fröhlich model [4]:



$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \sum_{\mathbf{k}}^{\Lambda} \hbar\omega_{\mathbf{k}} \hat{\alpha}^\dagger_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + \sum_{\mathbf{k}}^{\Lambda} V_{\mathbf{k}} e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} \left(\hat{\alpha}^\dagger_{-\mathbf{k}} + \hat{\alpha}_{\mathbf{k}}\right)$$

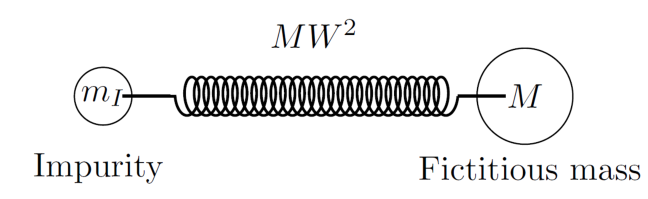
The Fröhlich Hamiltonian is encountered in many different polaronic systems, such as the optical polaron [4], the acoustic polaron [5], the ripplopolaron [6] and the more recent Bose polaron [7]. By integrating out the environment, the Fröhlich model can be equivalently described through an effective action functional for the impurity that now contains the memory effects:

$$\mathcal{S}_{\text{eff}}[\mathbf{r}(\tau)] = \frac{m}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau - \frac{1}{2}\sum_{\mathbf{k}} V_{\mathbf{k}}^2 \int_0^\beta d\tau \int_0^\beta d\sigma\, \mathcal{G}_{\mathbf{k}}(\tau-\sigma)\, e^{i\mathbf{k}\cdot[\mathbf{r}(\tau)-\mathbf{r}(\sigma)]}$$

Here, the second term describes the induced interaction of the impurity with itself as a consequence of integrating out the phonons. Unfortunately, even for the ground state properties of this effective action, no analytical solutions are known to exist.

Variational path integral treatment

Feynman's seminal idea [1,2] was to propose a simple analytical model action that could hopefully closely simulate the behavior of the difficult effective polaron action:



$$\mathcal{S}_0[\mathbf{r}(\tau)] = \frac{m}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau + \frac{MW^3}{8}\int_0^\beta d\tau \int_0^\beta d\sigma \frac{\cosh\left[W\left(u-\beta/2\right)\right]}{\sinh\left(W\beta/2\right)}\left[\mathbf{r}(\tau)-\mathbf{r}(\sigma)\right]^2$$

and then write down a variational inequality for the free energy of the effective action:

$$F < F_0 + \frac{1}{\beta}\left\langle \mathcal{S}_{\text{eff}} - \mathcal{S}_0 \right\rangle_0$$

This simple variational approach yields remarkable agreement with computationally demanding Diagrammatic Monte Carlo (DiagMC) calculations [8]:

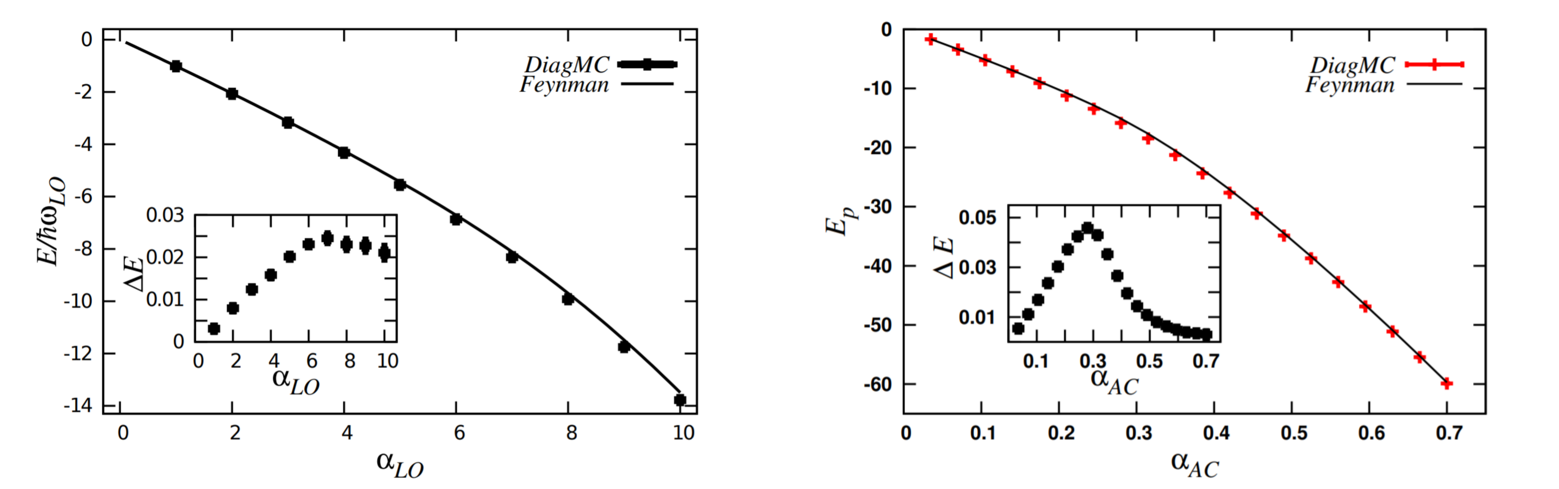


Fig. 1: The ground state energy of the Fröhlich model for the optical polaron (left) and the acoustic polaron (right) as a function of the coupling strength. Comparison between Feynman's result and DiagMC. Figure taken for illustrative purposes from [8].

Difficulties of the Bogoliubov-Fröhlich model

An impurity immersed in a Bose-Einstein condensate will form the Bose polaron. Similarly to other polaronic systems, at weak coupling the system can be described by the Fröhlich model, using [7]:

$$\omega_k \sim \sqrt{k^2(k^2+2)} \quad V_k \sim \left[k^2/(k^2+2)\right]^{1/4}$$

To a large surprise it was found that in this case, suddenly Feynman's approach fails to capture the behavior of the ground state energy, and even more powerful approaches yield some remaining discrepancies.

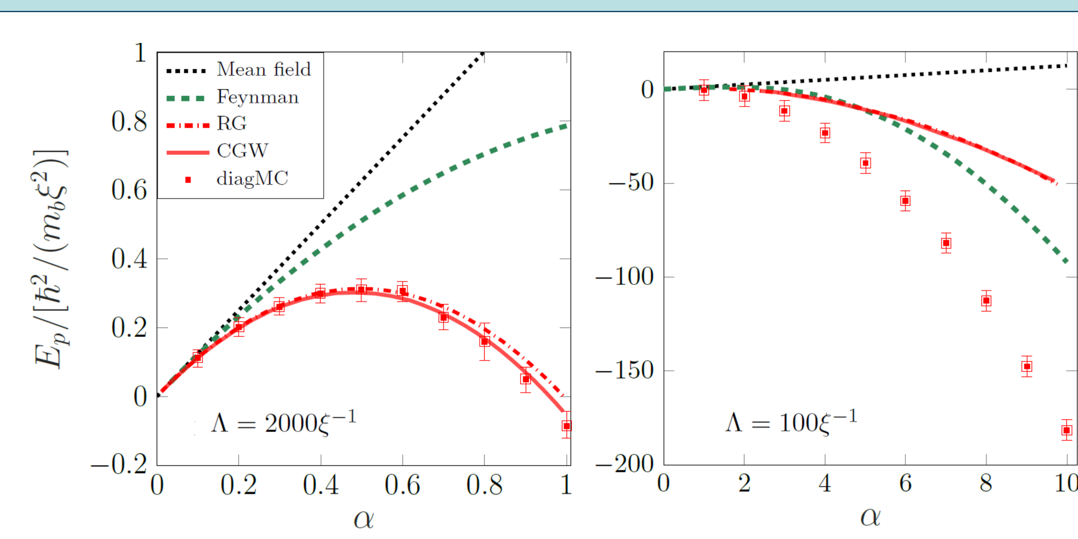
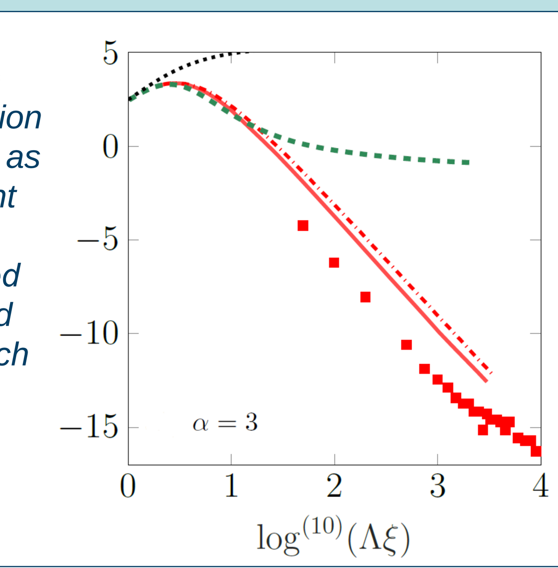


Fig. 2: The ground state energy of the Bogoliubov-Fröhlich model for as a function of the coupling strength (left panels) and as a function of the momentum cutoff (right panel). The green dashed line is Feynman's original approach [7], the red squares are DiagMC results [8], the red solid line is the Gaussian states approach [9], and the red dashed line is renormalization group theory [10].



Improving Feynman's approach

To tackle the Bogoliubov-Fröhlich model, two previously existing ideas have to be combined. First, we leave Feynman's oscillator model behind and follow [11] to consider the most general quadratic model action:

$$\mathcal{S}_0[\mathbf{r}(\tau)] = \frac{m}{2}\int_0^\beta \dot{\mathbf{r}}^2 d\tau + \frac{m}{2\beta}\int_0^\beta \int_0^\beta d\tau d\sigma\; x(\tau-\sigma)\mathbf{r}(\tau)\cdot\mathbf{r}(\sigma)$$

We find that this general memory kernel action is already capable of capturing the strong coupling limit of the Bogoliubov-Fröhlich model:

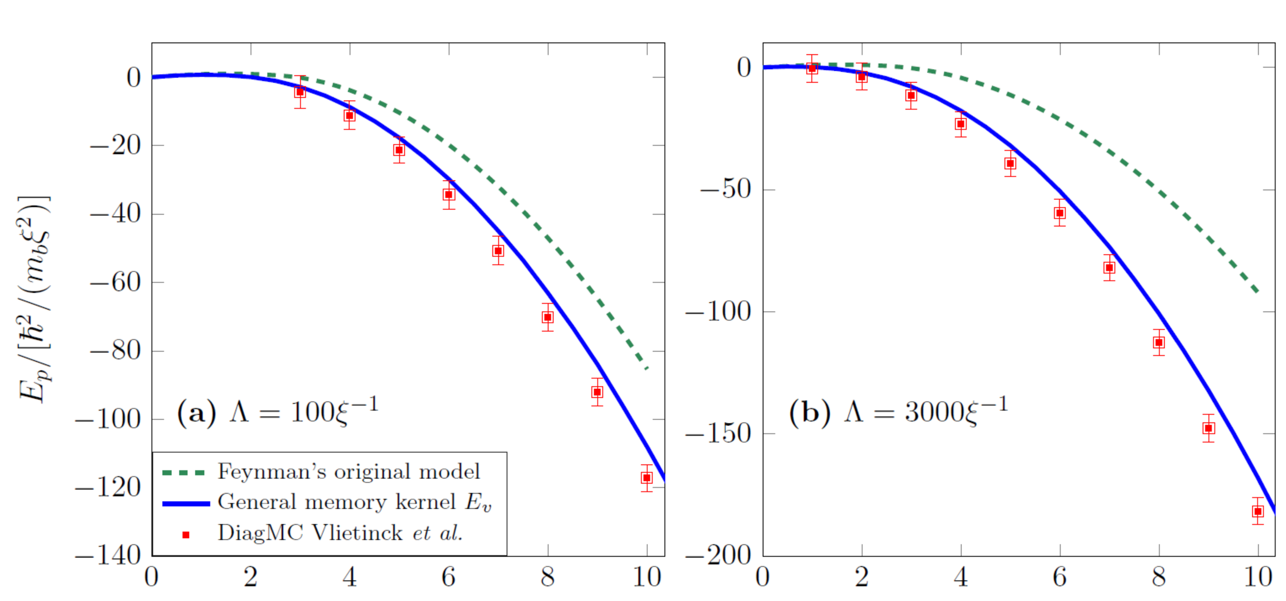


Fig. 3: The ground state energy of the Bogoliubov-Fröhlich model at strong coupling, comparing the general memory kernel approach (blue) with DiagMC (red).

However, at intermediate coupling it turns out that we still have to include corrections around the variational solution [12]:

$$F = F_0 + \frac{1}{\beta}\left\langle \Delta\mathcal{S}\right\rangle_0 - \frac{1}{2!}\frac{1}{\beta}\left\langle \left(\Delta\mathcal{S} - \left\langle\Delta\mathcal{S}\right\rangle\right)^2\right\rangle_0 + \mathcal{O}\left(\Delta\mathcal{S}^3\right)$$

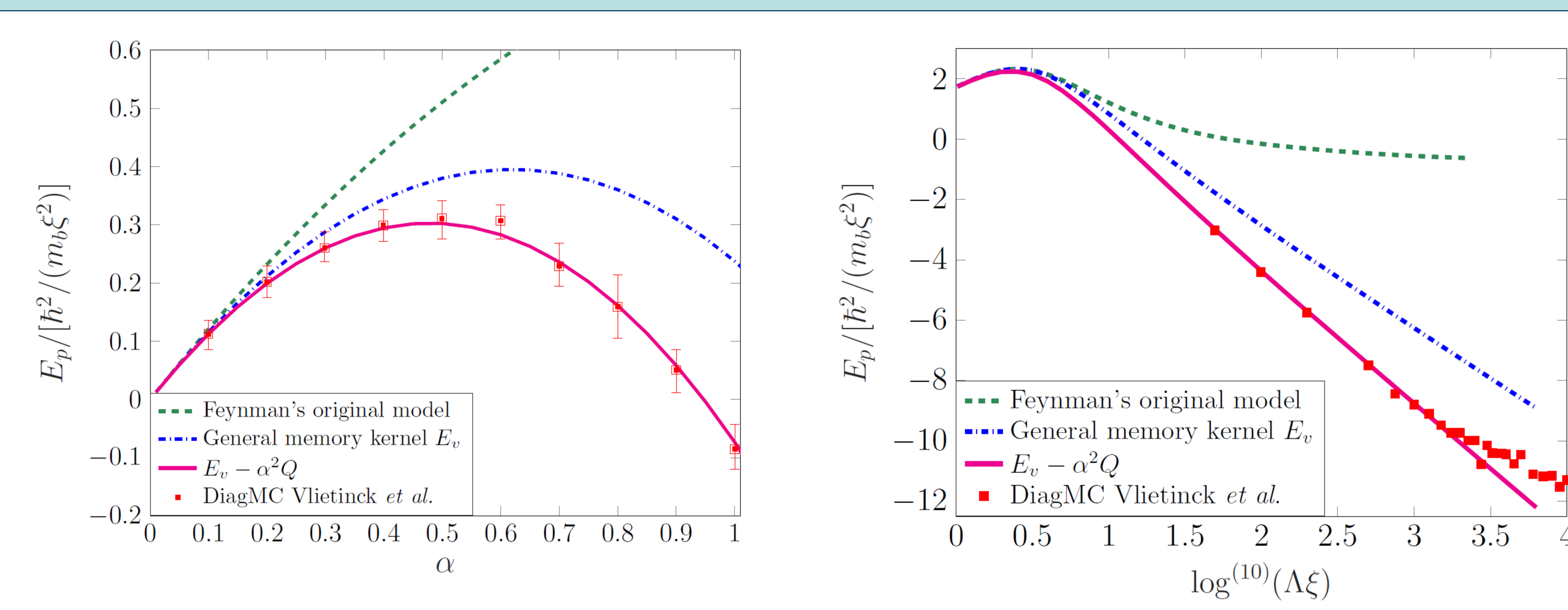


Fig. 4: The ground state energy of the Bogoliubov-Fröhlich model at weak to intermediate coupling (left panel) and as a function of the momentum cutoff (right panel), comparing the general memory kernel approach including perturbative corrections (magenta) with DiagMC (red).

Conclusion

The long-lasting supremacy of the variational path integral approach for the Fröhlich model has been recently questioned with the advent of the more exotic Bogoliubov-Fröhlich Hamiltonian in the context of the Bose polaron problem. It was found that Feynman's approach in its original formulation completely fails to capture the behavior of even the ground state energy.

In this work we have shown that by combining two previously existing ideas in the literature [11,12] and applying them to the Bogoliubov-Fröhlich model we obtain major improvements that provide excellent agreement with Diagrammatic Monte Carlo for this system. In doing so, we show that the path integral approach remains a powerful and versatile tool for polaronic physics.

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