1D Analogue of the Fröhlich Polaron Model Semiclassical Limit

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March 8, 2024

1 1D Polaron model [Sei20]

$$H_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \int \mathrm{d}k \, a_k^{\dagger} a_k - g \int \frac{\mathrm{d}k}{\sqrt{2\pi}} \left(a_k e^{ikx} + a_k^{\dagger} e^{-ikx} \right) \tag{1}$$

with $[a_k, a_{k'}^{\dagger}] = \delta(k - k')$. Note that by using different units $x \to g^{-2}x'$ and redefining the field variable $a_k \to gb_{g^{-2}k}$, we can scale out the q dependence:

$$H_g = -g^4 \frac{\mathrm{d}^2}{\mathrm{d}x'^2} + g^4 \int \mathrm{d}k \, b_k^{\dagger} b_k - g^4 \int \frac{\mathrm{d}k}{\sqrt{2\pi}} \left(b_k e^{ikx'} + b_k^{\dagger} e^{-ikx'} \right) = g^4 H \tag{2}$$

with $[b_k, b_{k'}^{\dagger}] = g^{-4}\delta(k - k')$. For strong coupling $g \to \infty$ the fields can be approximated by a classical function $\phi(x) = \int \frac{\mathrm{d}k}{\sqrt{2\pi}} b_k e^{ikx}$, since the $[b_k, b_{k'}^{\dagger}]$ commutator vanishes in this limit.

Energy functional $\mathbf{2}$

The expectation value of energy $\mathcal{E}(\psi, \phi) = \langle \psi | H | \psi \rangle$ becomes:

$$\mathcal{E}(\psi,\phi) = \int |\psi'|^2 + \int |\phi|^2 - \int |\psi|^2 (\phi + \phi^*)$$
(3)

and since we are interested in finding the ground state energy we can treat ϕ as a real-valued function, which sets the energy functional to:

$$\mathcal{E}(\psi,\phi) = \int |\psi'|^2 + \int \phi^2 - 2 \int |\psi|^2 \phi \tag{4}$$

Minimizing Eq. (4) over ϕ (note that it's just a quadratic function) sets $\phi_0 = |\psi|^2$ resulting in

$$\mathcal{E}(\psi) = \int |\psi'|^2 - \int |\psi|^4 \tag{5}$$

Minimizing Eq. (5) (by noting that the problem description matches that of a classical particle in a Mexican hat potential $V(q) = q^4 - \mu q^2$, where the μ term comes from the Lagrange multiplier setting constraint $\int |\psi|^2 = 1$ results in the ground state

$$\psi_0 = \frac{\sqrt{\mu}}{\cosh\left(\sqrt{\mu}x + C\right)} \text{ with } \mu = 1/4 \text{ to normalize the state}$$
(6)

and the ground state energy

$$\mathcal{E} = -1/12 \tag{7}$$

2.1 Mexican hat potential solution

Use energy conservation equation $\dot{q}^2 + q^4 - \mu q^2 = 0$ to deduce the trajectory:

$$\dot{q} = q\sqrt{\mu - q^2} \Rightarrow t + C_2 = \int \frac{\mathrm{d}q}{q\sqrt{\mu - q^2}} = \int \frac{\mathrm{d}p}{\mu - p^2} = \frac{\operatorname{arctanh}(p/\sqrt{\mu})}{\sqrt{\mu}} + C_1 \Rightarrow$$

$$\left| \text{where } p = \sqrt{\mu - q^2}; p\mathrm{d}p = q\mathrm{d}q \right| \Rightarrow q = \sqrt{\mu - \mu \tanh^2(\sqrt{\mu}t + C)} = \frac{\sqrt{\mu}}{\cosh(\sqrt{\mu}t + C)} \quad (8)$$

Now we are interested in field fluctuations around the minimum. We minimize Eq. (4) over ψ to obtain

$$\mathcal{E}(\phi) = \inf \operatorname{spec}(-\partial^2 - 2\phi) + \int \phi^2 \tag{9}$$

2.2 Expansion around the minimum

Using the non-degenerate second-order perturbation theory we calculate energy corrections up to the second order in $\delta\phi$. Note that since we expand around the minimum, the first-order contributions vanish.

$$H = H_0 + H_1 \tag{10}$$

$$|\psi\rangle = |\psi_0\rangle + |\psi_1\rangle + |\psi_2\rangle \tag{11}$$

$$E = E_0 + E_1 + E_2 \tag{12}$$

$$(H-E)|\psi\rangle = 0 \tag{13}$$

$$\downarrow (H_0 - E_0) |\psi_0\rangle + [(H_1 - E_1) |\psi_0\rangle + (H_0 - E_0) |\psi_1\rangle] + [(-E_2) |\psi_0\rangle + (H_1 - E_1) |\psi_1\rangle + (H_0 - E_0) |\psi_2\rangle] = 0$$
(14)

$$E_0 = \langle \psi_0 | H_0 | \psi_0 \rangle \tag{15}$$

$$|\psi_{0}\rangle \langle \psi_{0}| \left[(H_{1} - E_{1}) |\psi_{0}\rangle + (H_{0} - E_{0}) |\psi_{1}\rangle \right] = 0 \Rightarrow E_{1} = \langle \psi_{0}| H_{1} |\psi_{0}\rangle$$

$$\underbrace{(\mathbb{1} - |\psi_{0}\rangle \langle \psi_{0}|)}_{(H_{1} - E_{1}) |\psi_{0}\rangle + (H_{0} - E_{0}) |\psi_{1}\rangle}_{(H_{1} - E_{1}) |\psi_{0}\rangle + (H_{0} - E_{0}) |\psi_{1}\rangle}_{(H_{1} - E_{1}) |\psi_{0}\rangle + (H_{0} - E_{0}) |\psi_{1}\rangle} = 0 \Rightarrow$$

$$(16)$$

$$\frac{-|\psi_{0}\rangle\langle\psi_{0}|}{\mathbb{Q}}[(H_{1}-E_{1})|\psi_{0}\rangle+(H_{0}-E_{0})|\psi_{1}\rangle]=0 \Rightarrow$$
$$\Rightarrow \mathbb{Q}H_{1}|\psi_{0}\rangle=-\mathbb{Q}(H_{0}-E_{0})\mathbb{Q}|\psi_{1}\rangle\Rightarrow|\psi_{1}\rangle=-\frac{\mathbb{Q}}{H_{0}-E_{0}}H_{1}|\psi_{0}\rangle$$
(17)

 $|\psi_{0}\rangle \langle\psi_{0}| \left[(-E_{2}) |\psi_{0}\rangle + (H_{1} - E_{1}) |\psi_{1}\rangle + (H_{0} - E_{0}) |\psi_{2}\rangle \right] = 0 \Rightarrow E_{2} = \langle\psi_{0}| H_{1} |\psi_{1}\rangle = -\langle\psi_{0}| H_{1} \frac{\mathbb{Q}}{H_{0} - E_{0}} H_{1} |\psi_{0}\rangle$ (18)

3 Explicit form of the resolvent

Define $A = \partial + \frac{\psi'_0}{\psi_0}$. Then

$$AA^{\dagger} = \left(\partial + \frac{\psi_0'}{\psi_0}\right) \left(-\partial + \frac{\psi_0'}{\psi_0}\right) = -\partial^2 + \frac{\psi_0''}{\psi_0}$$
(20)

Since $(-\partial^2 - 2\psi_0^2 + 1/4)\psi_0 = 0$, we get $\frac{\psi_0''}{\psi_0} = -2\psi_0^2 + 1/4$. Therefore $AA^{\dagger} = H_0 - E_0$. Use polar decomposition to relate AA^{\dagger} and $A^{\dagger}A$

Use partial isometries to avoid the use of the projector \mathbb{Q} in the formula:

$$\frac{\mathbb{Q}}{H_0 - E_0} = \frac{\mathbb{Q}}{AA^{\dagger}} = U \frac{1}{A^{\dagger}A} U^{\dagger} = A \frac{1}{(A^{\dagger}A)^2} A^{\dagger}$$
(22)

where

$$A^{\dagger}A = \left(-\partial + \frac{\psi'_0}{\psi_0}\right) \left(\partial + \frac{\psi'_0}{\psi_0}\right) = -\partial^2 + 2\left(\frac{\psi'_0}{\psi_0}\right)^2 - \frac{\psi''_0}{\psi_0} = -\partial^2 + 1/4$$
(23)

For the final step note the commutation relation

$$A^{\dagger}\psi_{0} = \left(-\partial + \frac{\psi_{0}'}{\psi_{0}}\right)\psi_{0} = -\psi_{0}\partial$$

$$\tag{24}$$

Combining Eqs. (22) to (24) we get

$$\mathcal{E}(\phi_0 + \delta\phi) = -\frac{1}{12} + \langle \delta\phi | \,\mathbb{1} + 4\partial\psi_0 \frac{1}{\left(-\partial^2 + 1/4\right)^2} \psi_0 \partial \, |\delta\phi\rangle \tag{25}$$

Note that the eigenvalues of the operator $-\partial \psi_0 \frac{1}{(-\partial^2 + 1/4)^2} \psi_0 \partial$ lie in the range [0, 1/4] since $\mathcal{E} \ge -1/12$.

3.1 An eigenvector coming from translational invariance

To proper order in ε due to the translation invariance of the problem

$$\mathcal{E}(\phi_0 + \varepsilon \phi'_0) = \mathcal{E}(\phi_0) \tag{26}$$

Implying that $v_0 = \phi'_0$ is an eigenvector of $\mathcal{H} = -\partial \psi_0 \frac{1}{(-\partial^2 + 1/4)^2} \psi_0 \partial$ with eigenvalue 1/4.

3.1.1 Consistency checks

The following equalities hold (can be checked explicitly):

$$\psi_0 v_0 = (H_0 - E_0) \frac{1}{4} \frac{v_0}{\psi_0} = \left(-\partial^2 - 2\psi_0^2 + 1/4\right) \frac{1}{4} \frac{v_0}{\psi_0} \text{ with } \int \psi_0 \psi_0 v_0 = 0$$
(27)

$$-\psi_0 \partial v_0 = \left(-\partial^2 + 1/4\right)^2 \frac{1}{4}\psi_0 \tag{28}$$

$$-\partial\psi_0 \mathcal{F}^{-1} \frac{1}{(p^2 + 1/4)^2} \mathcal{F}\psi_0 \partial v_0 = \frac{1}{4} v_0 \text{ where } \mathcal{F} \text{ denotes Fourier transform } x \to p$$
(29)

4 Eigenvectors of \mathcal{H}

Writing an eigenvector as $v(x) = \partial_x g(x)$ equation $\mathcal{H}v = \lambda v$ becomes:

$$-\psi_0 \partial_x^2 g = \lambda \left(-\partial_x^2 + 1/4\right)^2 \frac{g}{\psi_0} \tag{30}$$

Note that both g(x) = 1 and g(x) = x solve Eq. (30):

$$(g(x) = 1) \quad \frac{1}{\psi_0} = 2\cosh(x/2) \Rightarrow \partial_x^2 \frac{1}{\psi_0} = \frac{1}{4} \cdot \frac{1}{\psi_0} \Rightarrow (-\partial_x^2 + 1/4)^2 \frac{1}{\psi_0} = (-1/4 + 1/4)^2 \frac{1}{\psi_0} = 0 \quad (31)$$

$$(g(x) = x) \quad \partial_x^2 \frac{x}{\psi_0} = 2\sinh(x/2) + \frac{1}{2}x\cosh(x/2) \Rightarrow \tag{32}$$

$$\Rightarrow (-\partial_x^2 + 1/4)^2 \frac{x}{\psi_0} = \sinh(x/2) + \frac{1}{8}x \cosh(x/2) - \left[\sinh(x/2) + \frac{1}{4}x \cosh(x/2)\right] + \frac{2}{16}x \cosh(x/2) = 0$$
(33)

The observation allows us to anticipate the absence of the zeroth g(x) and first-order $\partial_x g(x)$ terms in the equation, simplifying it from a fourth-order to a second-order differential equation. Expanding the right-hand side of Eq. (30) leads to a second-order equation for $\partial_x^2 g(x)$:

$$-\psi_0^2(x)g^{(2)}(x) = \lambda \left(g^{(2)}(x) + 2\tanh\left(\frac{x}{2}\right)g^{(3)}(x) + g^{(4)}(x)\right) \text{ where } g^{(n)}(x) = \partial_x^n g(x)$$
(34)

Changing variables to $h(x) = \partial_x^2 g(x)$ and $t = \tanh(x/2)$ Eq. (34) becomes:

$$(1 - t^2)\partial_t^2 h(t) + 2t \cdot \partial_t h(t) + \left[\frac{1}{\lambda} + \frac{4}{1 - t^2}\right]h(t) = 0$$
(35)

Equation (35) can be converted to the Legendre equation

$$(1 - t^2)\partial_t^2 y(t) - 2t \cdot \partial_t y(t) + n(n+1)y(t) = 0$$
(36)

by writing $h(x) = (1 - t^2)y(x)$ (note that we expect v(x) to rapidly decay at infinity, implying a vanishing value of h at $t = \pm 1$). Equation (35) transforms into:

$$(1-t^2)\partial_t^2 y(t) - 2t \cdot \partial_t y(t) + \left[\frac{1}{\lambda} + 2\right] y(t) = 0$$
(37)

The solution is spanned by $\mathsf{P}_{\frac{1}{2}\left(\sqrt{9+\frac{4}{a}}-1\right)}(t)$ and $\mathsf{Q}_{\frac{1}{2}\left(\sqrt{9+\frac{4}{a}}-1\right)}(t)$. The candidate eigenvalues are singled out by demanding $\frac{1}{\lambda} + 2 = n(n+1)$, which leads to $\frac{1}{2}\left(\pm\sqrt{9+\frac{4}{\lambda}}-1\right) = n$, which in turn implies

$$\lambda = \frac{4}{(2n+1)^2 - 9} = \frac{1}{(n-1)(n+2)}$$
(38)

4.1 Normalization

We require $g(|x| \to \infty) \to 0$ which in particular implies that

- 1. $\partial_x g(|x| \to \infty) = v(|x| \to \infty) \to 0 \Rightarrow v(|t| \to 1) \to 0 \Rightarrow \int_{-1}^1 \frac{2(1-t^2)y(t)}{1-t^2} dt = 0 \Rightarrow \int_{-1}^1 y(t) dt = 0.$ To show the penultimate relation we use $(1-t^2)y = h = \partial_x v = \frac{1-t^2}{2}\partial_t v$. Note that the polynomials P_k where $k \in \mathbb{N}$ satisfy the normalization constraint $\int_{-1}^1 \mathsf{P}_k(t) dt = 0$.
- $\begin{array}{ll} 2. \ \int_{-\infty}^{+\infty} \mathrm{d}x \, v(x) = 0 \Rightarrow \int_{-1}^{1} \mathrm{d}t \, \frac{1}{1-t^2} \int_{-1}^{t} \mathrm{d}u \, y(u) = 0 \Rightarrow \\ \Rightarrow \int_{-1}^{1} \mathrm{d}u \, y(u) \int_{u}^{1} \mathrm{d}t \, \frac{1}{1-t^2} = 0 \Rightarrow \int_{-1}^{1} \mathrm{d}u \, y(u) \mathrm{arctanh}(u) = 0 \ \mathrm{since} \ \int_{-1}^{1} y(t) \mathrm{d}t = 0. \end{array}$

Both conditions can be rewritten as orthogonality conditions:

$$\int_{-1}^{1} \mathrm{d}t \, y(t) \mathsf{P}_0(t) = 0 \tag{39}$$

$$\int_{-1}^{1} \mathrm{d}t \, y(t) \mathsf{Q}_0(t) = 0 \tag{40}$$

Since y(t) is a linear combination of $\mathsf{P}_k(t)$ and $\mathsf{Q}_k(t)$ to fulfill both Eqs. (39) and (40), it is sufficient to satisfy:

$$\left(\int \mathrm{d}t \,\mathsf{P}_k(t)\mathsf{Q}_0(t)\right) \left(\int \mathrm{d}t \,\mathsf{Q}_k(t)\mathsf{P}_0(t)\right) - \left(\int \mathrm{d}t \,\mathsf{P}_k(t)\mathsf{P}_0(t)\right) \left(\int \mathrm{d}t \,\mathsf{Q}_k(t)\mathsf{Q}_0(t)\right) = 0 \tag{41}$$

Using the inner product formulas for $P \cdot P$, $Q \cdot Q$ and $P \cdot Q$ (the links also include information about the formulas' scope):

$$\int_{-1}^{1} \mathsf{P}_{\nu}(x) \,\mathsf{P}_{\rho}(x) \,\mathrm{d}x = \frac{2 \left[2 \sin\left(\nu\pi\right) \sin\left(\rho\pi\right) \left(\psi_{\Gamma}\left(\nu+1\right) - \psi_{\Gamma}\left(\rho+1\right)\right) + \pi \sin\left((\rho-\nu)\pi\right)\right]}{\pi^{2}(\rho-\nu)(\rho+\nu+1)} \tag{42}$$

$$\int_{-1}^{1} \mathsf{Q}_{\nu}(x) \,\mathsf{Q}_{\rho}(x) \,\mathrm{d}x = \frac{(\psi_{\Gamma}(\nu+1) - \psi_{\Gamma}(\rho+1))(1 + \cos(\nu\pi)\cos(\rho\pi)) + \frac{1}{2}\pi\sin((\rho-\nu)\pi)}{(\rho-\nu)(\rho+\nu+1)} \tag{43}$$

$$\int_{-1}^{1} \mathsf{P}_{\nu}(x) \,\mathsf{Q}_{\rho}(x) \,\mathrm{d}x = \frac{2\sin\left(\nu\pi\right)\cos\left(\rho\pi\right)\left(\psi_{\Gamma}\left(\nu+1\right) - \psi_{\Gamma}\left(\rho+1\right)\right) + \pi\cos\left((\rho-\nu)\pi\right) - \pi}{\pi(\rho-\nu)(\rho+\nu+1)} \tag{44}$$

we reduce Eq. (41) to (remembering that we are looking for k > 0 solutions):

$$1 - \cos(\pi k) - \frac{2\sin(\pi k)}{\pi} [\psi_{\Gamma}(k+1) - \psi_{\Gamma}(1)] = 0$$
(45)

where $\psi_{\Gamma}(t) = \partial_t \ln(\Gamma(t)) = \frac{1}{\Gamma(t)} \partial_t \Gamma(t)$. Note that the positive even natural numbers $\{2, 4, \ldots\}$ clearly solve Eq. (45) as $1 - \cos(\pi 2q) = 0$ and $\sin(\pi 2q) = 0$ for $q \in \mathbb{N}$. The odd natural numbers work in the limit of large $k = 2t + 1 - \varepsilon$ where Eq. (45) reduces to $\mathcal{O}(\varepsilon^2) + 1 - (-1) - \frac{2}{\pi} \pi \varepsilon [\psi_{\Gamma}(k+1) - \psi_{\Gamma}(1)] = 0 \Leftrightarrow$ $\Leftrightarrow 1 - \varepsilon \ln(2t+2) \approx 0$. The other solutions come from a more intricate interplay between the digamma function ψ_{Γ} and the trigonometric functions.

4.2 Trace

Since all eigenvalues of \mathcal{H} are positive we can calculate the trace of \mathcal{H} to check if there are other eigenfunctions apart from the solutions of Eq. (45).

To separate out the integral kernel of ${\mathcal H}$ we write:

$$[\mathcal{H}f](y) = -\partial_y \psi_0(y) \frac{1}{2\pi} \int dp \, e^{-ipy} \int dx \, \frac{1}{(p^2 + 1/4)^2} e^{ipx} \psi_0(x) \partial_x f(x) = = \int dx \, \frac{1}{2\pi} \int dp \, \partial_y [\psi_0(y) e^{-ipy}] \partial_x [\psi_0(x) e^{ipx}] \frac{1}{(p^2 + 1/4)^2} f(x) = \int dx \, K(x, y) f(x) \quad (46)$$

where

$$K(x,y) = \frac{1}{2\pi} \int dp \,\partial_y [\psi_0(y)e^{-ipy}] \partial_x [\psi_0(x)e^{ipx}] \frac{1}{(p^2 + 1/4)^2}$$
(47)

$$\partial_{y}[\psi_{0}(y)e^{-ipy}]\partial_{x}[\psi_{0}(x)e^{ipx}] = \frac{1}{16}\frac{e^{ip(x-y)}}{\cosh(x/2)\cosh(y/2)}\left(\tanh(x/2)\tanh(y/2) + 2ip(\tanh(x/2) - \tanh(y/2)) + 4p^{2}\right)$$
(49)

For trace evaluation we need to compute K(x, x) which simplifies the integrals a bit, since the *p*-odd terms will vanish. Therefore we only need to evaluate the following two integrals: $\int dp \frac{p^{0/2}e^{ipx}}{(p^2+1/4)^2}$.

Using the appropriate semicircle contour (depending on the sign of x, to make sure the integrand decays at infinity) we obtain:

$$\int \mathrm{d}p \frac{e^{ipx}}{(p^2 + 1/4)^2} = 2\pi (2 + |x|)e^{-|x|/2} \tag{50}$$

$$\int \mathrm{d}p \frac{p^2 e^{ipx}}{(p^2 + 1/4)^2} = \pi (1 - |x|/2) e^{-|x|/2} = -\partial_x^2 \left[2\pi (2 + |x|) e^{-|x|/2} \right]$$
(51)

Combining Eqs. (49) to (51) and (55) we obtain:

$$K(x,x) = \frac{1}{2\pi} \frac{1}{16} \frac{1}{\cosh(x/2)^2} \left(\tanh(x/2)^2 + 1 \right) 4\pi = \frac{2\cosh(x/2)^2 - 1}{8\cosh(x/2)^4}$$
(52)

Using $\int \frac{1}{\cosh(x)^2} = \tanh(x) + C$ we compute

$$\int \mathrm{d}x \, K(x,x) = \frac{1}{2} \tanh(x/2)|_{-\infty}^{+\infty} - \frac{1}{4} \int \mathrm{d} \left[\tanh(x/2) \right] \left(1 - \left[\tanh(x/2) \right]^2 \right) = \left[\frac{1}{4} \tanh(x/2) + \frac{1}{12} \tanh(x/2)^3 \right] \Big|_{-\infty}^{+\infty} = \frac{2}{4} + \frac{2}{12} = \frac{2}{3} \quad (53)$$



Figure 1: The sum of the eigenvalues, obtained as positive solutions to Eq. (45), approaches the expected trace value of $\frac{2}{3}$.

Comparing the explicit trace value with the partial sums of the previously derived eigenvalues confirms their completeness, see Fig. 1.

Using the odd integral

$$\int \mathrm{d}p \frac{p \, e^{ipx}}{(p^2 + 1/4)^2} = i\pi x e^{-|x|/2} = -i\partial_x \left[2\pi (2 + |x|) e^{-|x|/2} \right] \tag{54}$$

we can also compute the off-diagonal entries of the integral kernel:

$$K(x,y) = \begin{cases} \frac{e^{y}(1+e^{x+y}-e^{x}(x-y))}{(1+e^{x})^{2}(1+e^{y})^{2}} & \text{if } x-y \ge 0\\ \frac{e^{x}(1+e^{x+y}+e^{y}(x-y))}{(1+e^{x})^{2}(1+e^{y})^{2}} & \text{else} \end{cases} = \frac{e^{\frac{x+y-|x-y|}{2}}(1+e^{x+y}-e^{x+y}|x-y|)}{(1+e^{x})^{2}(1+e^{y})^{2}} \tag{55}$$

Equation (55) allows us to compute not only the tr[\mathcal{H}] = $\int dx K(x, x) = \sum_{\lambda_i \in \text{spec}(\mathcal{H})} \lambda_i$, but also the tr[\mathcal{H}^2] = $\sum_{\lambda_i \in \text{spec}(\mathcal{H})} \lambda_i^2 = \int dx \int dy K(x, y)^2$:

1. For $x \ge y$ the kernel becomes $K(x,y) = \frac{e^y}{(1+e^x)^2(1+e^y)^2} (1+e^{x+y}-(x-y)e^x)$

2.

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{x} dy \, K(x,y)^2 = \frac{\pi^2 - 5}{108}$$

3. Using the symmetry of the kernel K(x, y) = K(y, x) we conclude

$$\int_{-\infty}^{\infty} dy \int_{-\infty}^{y} dx \, K(x,y)^2 = \int_{-\infty}^{\infty} dy \int_{-\infty}^{y} dx \, K(y,x)^2 = \frac{\pi^2 - 5}{108}$$
(56)

Summing up the integrals over the $x \ge y$ and $x \le y$ regions we get:

$$tr[\mathcal{H}^2] = \int dx \int dy \, K(x,y)^2 = \frac{\pi^2 - 5}{54}$$
(57)

5 Complex analysis approach to finding the sum of function roots

While we were able to obtain the first and second moments of \mathcal{H} by explicitly integrating its integral kernel, this method does not generalize well for higher moments. Instead, we can directly compute sums (of functions) of solutions to Eq. (45). The idea is to use the argument principle applied to the left-hand side of Eq. (45) together with Eq. (38), since both expressions are explicit:

$$\frac{1}{2\pi i} \int_C \mathrm{d}z \, \frac{F'(z)}{F(z)} h^k(z) = \sum_{z_i \in \text{ zeros of } F \text{ in } C} [\mathrm{multiplicity}(z_i)] h^k(z_i) + \mathrm{res}_{z=1} \frac{F'(z)}{F(z)} h^k(z) \tag{58}$$



Figure 2: The horizontal parts of the integration contour C extend to $\pm i\infty$ and connect at $+\infty$. Dark dots denote (simple) zeros of F, the dark square at z = 0 highlights F's zero with multiplicity 2. The cross at z = 1 shows the relevant (contained in C) pole of h^k . Gray dashes between 1 and 2 indicate the branch cut of the function j. The white circles emphasize the important symmetry: F, h^k, j are even about $-\frac{1}{2}$, i.e. $F(-\frac{1}{2}+z) = F(-\frac{1}{2}-z)$.

where

$$F(z) = 1 - \cos(\pi z) - \frac{2\sin(\pi z)}{\pi} [\psi_{\Gamma}(z+1) - \psi_{\Gamma}(1)] \qquad h^k(z) = \frac{1}{(z-1)^k (z+2)^k}$$
(59)

and the contour C is shown in orange on Fig. 2.

We expect the integral \int_C to vanish since its argument decays fast enough at infinities and it is odd (both together with $h^k(z)$ and j(z)) about $-\frac{1}{2}$, so the integral along $\Re(z) = 0$ is also zero.

$$|F'(z)| \xrightarrow[|z|\to\infty,\cos(\pi z)\sim1]{} |2\cos(\pi z)\ln(z)| \quad |F(z)| \xrightarrow[|z|\to\infty,\sin(\pi z)\sim1]{} \left|\frac{2\sin(\pi z)}{\pi}\ln(z)\right| \quad |[j/h](z)| \xrightarrow[|z|\to\infty]{} \frac{1}{|z|\to\infty} (60)$$

Splitting out the irrelevant contribution at z = 0 we therefore obtain:

$$0 = \operatorname{res}_{z=0} \frac{F'(z)}{F(z)} h^k(z) + \operatorname{res}_{z=1} \frac{F'(z)}{F(z)} h^k(z) + \sum_{\lambda_i \in \operatorname{spec}(\mathcal{H})} \lambda_i^k$$
(61)

Recalling the residue formula for an n-th-order pole:

$$\operatorname{res}_{z=z_0} f = \lim_{z \to z_0} \frac{1}{(n-1)!} \partial_z^{n-1} (z-z_0)^n f(z)$$
(62)

we directly compute the residue at z = 0 (here n = 2):

$$\operatorname{res}_{z=0} \frac{F'(z)}{F(z)} h^k(z) = \lim_{z \to 0} \frac{6}{\pi^2} \partial_z F'(z) h^k(z) = -\left(-\frac{1}{2}\right)^{k-1}$$
(63)

where we used $F(\varepsilon) = 1 - \left(1 - \frac{(\pi\varepsilon)^2}{2}\right) - \frac{2}{\pi}\pi\varepsilon\frac{\pi^2}{6}\varepsilon + \mathcal{O}(\varepsilon^3) = \frac{\pi^2}{6}\varepsilon^2 + \mathcal{O}(\varepsilon^3)$. For the other residue we should use Eq. (62) with n = k, so it's not easy to obtain a simple expression for general k. But it can be done for specific choices of k, e.g. $\operatorname{res}_{z=1}\frac{F'(z)}{F(z)}h^1(z) = \frac{1}{3}$ and $\operatorname{res}_{z=0}\frac{F'(z)}{F(z)}h^1(z) = -1$ imply (via Eq. (61))

$$\sum_{\lambda_i \in \operatorname{spec}(\mathcal{H})} \lambda_i = \frac{2}{3} \tag{64}$$

while $\operatorname{res}_{z=1} \frac{F'(z)}{F(z)} h^2(z) = -\frac{22+\pi^2}{54}$ and $\operatorname{res}_{z=0} \frac{F'(z)}{F(z)} h^2(z) = \frac{1}{2}$ imply $\sum_{\lambda_i \in \operatorname{spec}(\mathcal{H})} \lambda_i^2 = \frac{\pi^2 - 5}{54}$

which are consistent with the results previously obtained from the explicit expression of the integral kernel of \mathcal{H} .

Sums $\sum_{\lambda_i \in \text{spec}(\mathcal{H})} \lambda_i^k$ for larger k start including higher-order derivatives of log-gamma function, but the expressions are accessible if needed.

To compute the order $\mathcal{O}(g^0)$ ground state energy correction we have to compute the sum from the second term in Eq. (71). Using

$$j(z) = \sqrt{\frac{1}{4} - \frac{1}{(z-1)(z+2)}} - \frac{1}{2}$$
(66)

(65)

instead of $h^k(z)$ we obtain an equation analogous to Eq. (61), by noting that the square root $\sqrt{\frac{1}{4} - \frac{1}{(z-1)(z+2)}}$ introduces a branch cut at the negative values of its argument $\frac{1}{4} - \frac{1}{(z-1)(z+2)} < 0 \Leftrightarrow z \in (1,2) \cup (-3,-2)$:

$$0 = \operatorname{res}_{z=0} \frac{F'(z)}{F(z)} j(z) - \frac{1}{2\pi i} \int_{1}^{2} \mathrm{d}z \operatorname{disc} \left[\frac{F'(z)}{F(z)} j(z) \right] + \sum_{\lambda_{i} \in \operatorname{spec}(\mathcal{H})} \left[\sqrt{1/4 - \lambda_{i}} - 1/2 \right]$$
(67)

where disc $[G(z)] = \lim_{\varepsilon \to 0} G(z + i\varepsilon) - G(z - i\varepsilon).$

For the residue term we obtain:

$$\operatorname{res}_{z=0} \frac{F'(z)}{F(z)} j(z) = \lim_{z \to 0} \frac{6}{\pi^2} \partial_z F'(z) j(z) = \sqrt{3} - 1$$
(68)

Discontinuity of the square root is disc $[\sqrt{z}]_{|z||_{z=0}} = 2i\sqrt{|z|}$, therefore

$$\frac{1}{2\pi i} \int_{1}^{2} \mathrm{d}z \operatorname{disc} \left[\frac{F'(z)}{F(z)} j(z) \right] = \frac{1}{2\pi i} \int_{1}^{2} \mathrm{d}z \frac{F'(z)}{F(z)} \operatorname{disc} \left[j(z) \right] = \frac{1}{\pi} \int_{1}^{2} \mathrm{d}z \frac{F'(z)}{F(z)} \sqrt{\left| \frac{1}{4} - \frac{1}{(z-1)(z+2)} \right|} \approx -0.22291 \quad (69)$$

Combining both results with Eq. (67) we get

$$\sum_{\lambda_i \in \text{spec}(\mathcal{H})} \left[\sqrt{1/4 - \lambda_i} - 1/2 \right] \approx -0.22291 - (\sqrt{3} - 1) \approx -0.95496$$
(70)

6 Order $\mathcal{O}(g^0)$ energy correction

The next-order quantum correction to the ground state energy can be expressed in terms of the eigenvalues of \mathcal{H} , and the direct numerical summation gives (matching the complex analysis numerics):

$$\mathcal{E}_g = -\frac{1}{12}g^4 + \sum_{\lambda_i \in \text{spec}(\mathcal{H})} \left[\sqrt{1/4 - \lambda_i} - 1/2\right] \approx -\frac{1}{12}g^4 - 0.95496$$
(71)

6.1 Quantum correction derivation

Recall the initial Hamiltonian Eq. (1) where the first (kinetic) term has been relabeled into momentum squared $P_{\rm cl}^2$, the second (field energy) term has been rewritten in terms of local position $Q_x = \frac{a_x^{\dagger} + a_x}{\sqrt{2}}$ and conjugate momentum $P_x = i \frac{a_x^{\dagger} - a_x}{\sqrt{2}}$ operators, and the third term represents the potential $V_{\rm cl}[Q]$ that the electron feels in the adiabatic approximation.

$$H_g = P_{\rm cl}^2 + \int \mathrm{d}x \, \left(\frac{P_x^2 + Q_x^2}{2} - \frac{1}{2}\right) + V_{\rm cl}[Q] \tag{72}$$

Using $Q_x = \sqrt{2}\phi(x)$ and disregarding lower order $o\left((Q/\sqrt{2}-\phi_0)^2\right)$ terms we obtain (using Eq. (25)):

$$P_{\rm cl}^2 + V_{\rm cl}[Q] + \int \mathrm{d}x \,\phi(x)^2 = P_{\rm cl}^2 + V_{\rm cl}[Q] + \frac{1}{2} \int \mathrm{d}x \,Q_x^2 = -\frac{1}{12}g^4 + \left\langle Q/\sqrt{2} - \phi_0 \right| \,\mathbb{1} - 4\mathcal{H} \left| Q/\sqrt{2} - \phi_0 \right\rangle \tag{73}$$

Plugging back into Eq. (72) we get:

$$\inf \operatorname{spec}(H_g) = \inf \operatorname{spec}\left(-\frac{1}{12}g^4 + \int \mathrm{d}x \left(\frac{P_x^2 + Q_x[\mathbbm{1} - 4\mathcal{H}]Q_x}{2} - \frac{1}{2}\right)\right) = \\ = -\frac{1}{12}g^4 + \int \mathrm{d}x \left\langle Q_x \left| \frac{\sqrt{\mathbbm{1} - 4\mathcal{H}} - \mathbbm{1}}{2} \right| Q_x \right\rangle = -\frac{1}{12}g^4 + \int \mathrm{d}x \left\langle Q_x \left| \sqrt{\frac{\mathbbm{1}}{4} - \mathcal{H}} - \frac{\mathbbm{1}}{2} \right| Q_x \right\rangle \quad (74)$$

7 First few excitation energies



Figure 3: Normalizable solutions of Eq. (75).

8 Numerics

Writing an eigenvector as $v(x) = (\psi_0 y(x))'$ equation $\mathcal{H}v = \lambda v$ becomes:

$$-\psi_0(\psi_0 y)'' = \lambda \left(-\partial^2 + 1/4\right)^2 y \text{ where } \lambda \text{ is the eigenvalue}$$
(75)

8.1 $\lambda = 0$

The full solution is

$$y(x) = \frac{C_1 x + C_2}{\psi_0(x)} \text{ with } v(x) = C_1 \text{ (no normalizable choices of } v)$$
(76)

8.2 $\lambda = 1$

A solution is given by

$$y = \psi_0 \text{ with } v = (\psi_0^2)'$$
 (77)

Numerical solutions of Eq. (75) with initial conditions at x = 0 taken from the solution $y = \psi_0$, i.e. y(0) = 0.5, y'(0) = 0, y''(0) = -0.125, y'''(0) = 0 result in normalizable $v = (\psi_0 y)'$ only for certain values of λ . The eigenvalue sequence decays according to a power law $\sim \frac{1}{n^2}$.

The list of the first few values:

$$\frac{1}{4}; \frac{1}{18}; \frac{1}{40}; \frac{1}{70}; \frac{1}{108}; \frac{1}{154}; \frac{1}{208}; \dots$$



Figure 4: Roots of $v_{\infty}(\lambda)$ are the values of λ that result in a normalizable eigenfunction. Here the definition for v_{∞} reads as $v_{\infty} = v(x = 90)$; note that the point $x_0 = 90$ is chosen to satisfy the condition $v'(x > x_0) = 0$.



Figure 5: Power law decay of 4λ

9 Understanding \mathcal{H}

$$\mathcal{F}[x^n] = \frac{1}{\sqrt{2\pi}} \int_x e^{ipx} x^n = \sqrt{2\pi} \left(-i\partial_p\right)^n \delta(p) \tag{78}$$

Analogously

$$\mathcal{F}^{-1}\frac{1}{(p^2+1/4)^2}\mathcal{F}[x^n] = (i\partial_p)^n \frac{e^{-ipx}}{(p^2+1/4)^2}|_{p=0} = (-i\partial_p)^n \frac{e^{ipx}}{(p^2+1/4)^2}|_{p=0}$$
(79)

$$\mathcal{F}[\sin(x)] = \frac{1}{\sqrt{2\pi}} \int_{x} e^{-ipx} \frac{e^{ix} - e^{-ix}}{2i} = \sqrt{\frac{\pi}{2}} i \left[\delta(p-1) - \delta(p+1)\right]$$
(80)

$$\mathcal{F}^{-1}\frac{1}{(p^2+1/4)^2}\mathcal{F}[\sin(x)] = \frac{1}{(1^2+1/4)^2}\sin(x) = \frac{16}{25}\sin(x) \tag{81}$$

$$\mathcal{F}^{-1}\frac{1}{(p^2+1/4)^2}\mathcal{F}[\cos(x)] = \frac{1}{(1^2+1/4)^2}\cos(x) = \frac{16}{25}\cos(x)$$
(82)

$$\mathcal{F}^{-1}\frac{1}{(p^2+1/4)^2}\mathcal{F}[\sin(ax)] = \frac{1}{(a^2+1/4)^2}\sin(x) = \frac{16}{(4a^2+1)^2}\sin(x) \tag{83}$$

$$\mathcal{F}^{-1}\frac{1}{(p^2+1/4)^2}\mathcal{F}[\cos(ax)] = \frac{1}{(a^2+1/4)^2}\cos(x) = \frac{16}{(4a^2+1)^2}\cos(x) \tag{84}$$

References

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