Non-polynomial phonon action for a dimer with one electron

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Abstract. The partition function of a dimer with one electron, interacting with two local Einstein phonons, is reduced to the pure phonon partition function. It is investigated analytically in the coherent-state path-integral representation in order to recognize the competition between electron hopping and electron–phonon interaction. The non-polynomial term in the phonon action, promoted by electron hopping, is deduced. The low-temperature resonance decoupling between electron and phonon systems destroys the low-temperature tendency of electron localization in the case of small hopping and large electron–phonon coupling. The comparison with polaronic theory is completed.

1. Introduction

The polaron—a bound state of a conducting electron and phonon—is a fundamental concept in electron–phonon interaction theory when the constant g of electron–phonon interaction is large enough [1]. It is known that the phonon and polaron degrees of freedom can be decoupled in zero order of $1/g$ perturbation theory [2]. The formation of the polaron changes the thermodynamics and the conducting properties of a crystal as well as the lattice distortion.

In molecular crystal in the general case a conducting electron interacts with inter- and intra-site phonons [3]. In the last few years interest has been shown in Holstein-type models of molecular crystals and clusters in terms of a general interest in systems with a small number of particles. Numerical calculations are performed for ground state properties in these cases [4–6]. The simplest version of such a system is the Holstein dimer with a single electron, interacting with the site Einstein phonons, while the inter-molecular oscillations are neglected.

This two-site model with one electron has been the topic of a lot of research [7] which has used the polaron representation for an electron and phonons of the dimer. This model is also the subject of the present work. In contrast to the quoted papers, we use an analytical description and evaluate the partition function of a dimer in the thermal equilibrium state. Via the averaging over the electron variable we find a non-polynomial effective phonon Hamiltonian that leads to a path-integral representation for the partition function. This treatment is similar to the adiabatic approach for electrons and nuclei in molecules. We consider the competition between the electron hopping t and electron–phonon interaction g, since the phonon action depends on the parameter t after extracting the electron variables. Our idea is to return to the initial quantum-statistical images with the purpose of creating

an additional picture for the conditions of polaron existence. In particular, we obtain the resonance values of phonon parameters, where the electron and phonon variables can be decoupled. Also, we demonstrate the tendency for high-temperature localization of the electron. We do not use the polaronic picture, but we can compare the result of nonlinear phonon dynamics with some conclusions from the ordinary polaronic treatment.

2. Phonon system for symmetric and antisymmetric electron states

Let us start with the Hamiltonian

$$H = -t(c_1^+ c_2 + c_2^+ c_1) + \Omega(a_1^+ a_1 + a_2^+ a_2) + g(a_1^+ + a_1)n_1 + g(a_2^+ + a_2)n_2 - \mu(n_1 + n_2) \tag{1}$$

where c_i^+ (c_i) is the creation (annihilation) operator of an electron at site $i = 1, 2$ (we drop the spin subscript), $n_i = c_i^+ c_i$, a_i^+ (a_i) is the creation (annihilation) operator of a phonon of frequency Ω at site i, t is the electron-hopping constant and μ is the one-particle level.

We search for a wavefunction of the Hamiltonian (1) in the following form:

$$\Psi = c_1^+ f_1(a_1^+, a_2^+)|0\rangle^{\text{el}}|0\rangle^{\text{ph}} + c_2^+ f_2(a_1^+, a_2^+)|0\rangle^{\text{el}}|0\rangle^{\text{ph}} \tag{2}$$

where

$$|0\rangle^{\text{el}} = |0\rangle_1^{\text{el}}|0\rangle_2^{\text{el}} \qquad |0\rangle^{\text{ph}} = |0\rangle_1^{\text{ph}}|0\rangle_2^{\text{ph}}.$$

After the substitution of (2) into the Schrödinger equation $H\Psi = E\Psi$ we equate the phonons' operator coefficients at the electron basis functions $c_1^+|0\rangle^{\text{el}}$ and $c_2^+|0\rangle^{\text{el}}$. With the use of the relations $n_i c_j^+|0\rangle^{\text{el}} = \delta_{ij} c_j^+|0\rangle^{\text{el}}$ we derive two equations, which may be represented in a matrix form:

$$\begin{pmatrix} \hat{\Omega}_1 - E - \mu & -t \\ -t & \hat{\Omega}_2 - E - \mu \end{pmatrix} \begin{pmatrix} f_1(a_1^+, a_2^+)|0\rangle^{\text{ph}} \\ f_2(a_1^+, a_2^+)|0\rangle^{\text{ph}} \end{pmatrix} = 0 \tag{3}$$

$$\hat{\Omega}_i = \Omega(a_1^+ a_1 + a_2^+ a_2) + g(a_i^+ + a_i).$$

Our next step is the diagonalization of the operator matrix (3). Let us consider the transformation $\mathbf{U}$,

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \hat{P}_{12} \\ 1 & -\hat{P}_{12} \end{pmatrix} \qquad \mathbf{U}^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ \hat{P}_{12} & -\hat{P}_{12} \end{pmatrix}$$

where $\hat{P}_{12}$ permutates the symbols a_1^+ and a_2^+. Really, the operators $\hat{\Omega}_{1(2)}$ and $\hat{P}_{12}$ do not commute; they obey the equations $\hat{P}_{12}\hat{\Omega}_{1(2)} = \hat{\Omega}_{2(1)}\hat{P}_{12}$, $\hat{P}_{12}^2 = 1$. Using these relations, one can easily check that

$$\mathbf{U}\begin{pmatrix} \hat{\Omega}_1 - E - \mu & -t \\ -t & \hat{\Omega}_2 - E - \mu \end{pmatrix}\mathbf{U}^{-1} = \begin{pmatrix} H_- - E & 0 \\ 0 & H_+ - E \end{pmatrix}$$

$$H_- = \Omega(a_1^+ a_1 + a_2^+ a_2) + g(a_1^+ + a_1) - t\hat{P}_{12} - \mu$$

$$H_+ = \Omega(a_1^+ a_1 + a_2^+ a_2) + g(a_2^+ + a_2) + t\hat{P}_{12} - \mu.$$

In essence, the transformation $\mathbf{U}$ is a kind of Fulton–Gouterman transformation [8]. Now the Schrödinger equation (3) looks like

$$\begin{pmatrix} H_- - E & 0 \\ 0 & H_+ - E \end{pmatrix}\mathbf{U}\begin{pmatrix} f_1(a_1^+, a_2^+)|0\rangle^{\text{ph}} \\ f_2(a_1^+, a_2^+)|0\rangle^{\text{ph}} \end{pmatrix} = 0 \tag{4}$$

where the column of the phonons' vectors is transformed in the following way:

$$
\mathsf{U} \begin{pmatrix} f_1(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} \\ f_2(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} \end{pmatrix} = \begin{pmatrix} F_s(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} \\ F_a(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} \end{pmatrix}
$$

$$
= \frac{1}{\sqrt{2}} \begin{pmatrix} f_1(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} + \hat{P}_{12}\, f_2(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} \\ f_1(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} - \hat{P}_{12}\, f_2(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} \end{pmatrix}
$$

$$
= \frac{1}{\sqrt{2}} \begin{pmatrix} f_1(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} + f_2(a_2^+, a_1^+)|0\rangle^{\mathrm{ph}} \\ f_1(a_1^+, a_2^+)|0\rangle^{\mathrm{ph}} - f_2(a_2^+, a_1^+)|0\rangle^{\mathrm{ph}} \end{pmatrix}.
$$

Now one can see that the wavefunction (2) may be written in a form

$$
\Psi = \left[\tfrac{1}{2}(c_1^+ + c_2^+ \hat{P}_{12})\, F_s(a_1^+, a_2^+) + \tfrac{1}{2}(c_1^+ - c_2^+ \hat{P}_{12})\, F_a(a_1^+, a_2^+) \right]|0\rangle^{\mathrm{ph}}|0\rangle^{\mathrm{el}}
$$

which represents the symmetric and antisymmetric electron states, taking account of the phonon permutation symmetry. This means that the spectrum of the initial system (1) coincides with the superposition of the spectra of the Schrödinger equations for the phonon wavefunctions F_s and F_a with eigenvalues $E_\mp$, which originate from the symmetric and antisymmetric electron states

$$
H_- F_s = E_- F_s \qquad H_+ F_a = E_+ F_a.
$$

Therefore, the partition function of the system (1) may be calculated as

$$
Z = \mathrm{Sp}\, e^{-\beta H} = Z_+ + Z_- = \mathrm{sp}\, e^{-\beta H_+} + \mathrm{sp}\, e^{-\beta H_-}
$$

$$
Z_+(t) = Z_-(-t) \tag{5}
$$

where Sp means the trace over phonon and electron variables, while sp means the trace over phonon variables only. The operator $\hat{P}_{12}$ acting on the boson basic vectors is deduced in the appendix in terms of operators a_1, a_2, a_1^+, a_2^+

$$
P_{12} = \cos\left[\tfrac{1}{2}\pi(-a_1^+ a_1 - a_2^+ a_2 + a_1^+ a_2 + a_2^+ a_1) \right]. \tag{6}
$$

3. Path integral for phonon partition function

In order to evaluate the partition function $Z_\mp$ for Hamiltonians $H_\mp$ with the operator form (6) we take $Z_\mp$ as the path integrals in the Bose-coherent representation

$$
Z_\mp = \int Da_1^* \, Da_1 \, Da_2^* \, Da_2 \, \exp(S_\mp). \tag{7}
$$

The part of the action $S_\mp$ corresponding to the operator $\hat{P}_{12}$ can be calculated directly from the limiting procedure for the path integral. The decomposition of unity has the following form:

$$
\hat{I} = \int \prod_{i=1,2} d\mu_i \, (|z_i\rangle_i \,_i\langle z_i|)
$$

where $|z\rangle$ are the usual Klauder coherent states. Then, for the $N \sim \infty$ time-sliced matrix elements approximation [9] we have

$$
{}_2\langle z'_{i+1}|{}_1\langle z_{i+1}| \exp\left[\frac{\beta t \hat{P}}{N}\right]|z_i\rangle_1|z'_i\rangle_2 \sim {}_2\langle z'_{i+1}|{}_1\langle z_{i+1}| 1 + \frac{\beta t \hat{P}}{N} |z_i\rangle_1|z'_i\rangle_2
$$

$$
= {}_2\langle z'_{i+1}|z'_i\rangle_2 \,_1\langle z_{i+1}|z_i\rangle_1 \left(1 + \frac{t}{N} \frac{{}_2\langle z'_{i+1}|z_i\rangle_2 \,_1\langle z_{i+1}|z'_i\rangle_1}{{}_2\langle z'_{i+1}|z'_i\rangle_2 \,_1\langle z_{i+1}|z_i\rangle_1} \right)
$$

$$
= {}_2\langle z'_{i+1}|z'_i\rangle_2 \,_1\langle z_{i+1}|z_i\rangle_1 \left(1 + \frac{\beta t}{N} \exp(z_i \bar{z}'_{i+1} + z'_i \bar{z}_{i+1} - z'_i \bar{z}'_{i+1} - z_i \bar{z}_{i+1}) \right).
$$

So, the actions for $Z_{\mp}$ are as follows:

$$S_{\mp} = -\int_0^{\beta} [\bar{a}_1 \dot{a}_1 + \bar{a}_2 \dot{a}_2 + \Omega(\bar{a}_1 a_1 + \bar{a}_2 a_2) + g(\bar{a}_1 + a_1)$$

$$\mp t \exp(-\bar{a}_1 a_1 - \bar{a}_2 a_2 + \bar{a}_1 a_2 + \bar{a}_2 a_1)]\,d\tau.$$

It is convenient to change the variables

$$a_2 = \frac{u+v}{\sqrt{2}} \qquad a_1 = \frac{v-u}{\sqrt{2}} \tag{8}$$

and to get the action in the form:

$$S_{\mp} = -\int_0^{\beta} \left[\bar{u}\dot{u} + \bar{v}\dot{v} + \Omega(\bar{u}u + \bar{v}v) + \frac{g}{\sqrt{2}}(\bar{v} + v - \bar{u} - u) \mp t\exp(-2\bar{u}u) \right] d\tau.$$

The factorization of $Z_{\mp}$ takes place in the variables u and v and we can write $S_{\mp} = S_v + S_{\mp u}$ and correspondingly, $Z_{\mp} = Z_v Z_{\mp,u}$. The integral over v-variables is Gaussian and can be calculated explicitly, so that

$$Z = \exp\left(\beta\left(\mu + \frac{g^2}{2\Omega} \right) \right) \frac{1}{1 - \exp(-\beta\Omega)} \int D\bar{u}\, Du \exp S_{\pm,u}$$

where

$$S_{\pm,u} = -\int_0^{\beta} \left[\bar{u}\dot{u} + \Omega\bar{u}u - \frac{g}{\sqrt{2}}(\bar{u} + u) \pm t\exp(-2\bar{u}u) \right] d\tau. \tag{9}$$

It is impossible to calculate the integral over u in (7) explicitly, and we try to choose an approximation scheme taking into account the exact solutions for particular cases. For $t = 0$,

$$Z_{\mp}|_{t=0} = e^{\beta\mu} \frac{\exp(\beta g^2/\Omega)}{(1 - \exp(-\beta\Omega))^2} \qquad Z|_{t=0} = 2Z_{\mp}|_{t=0}. \tag{10}$$

The partition function Z in the limiting case $g = 0$ can be easily calculated since we have a non-interacting electron and phonons. Evaluation of each of $Z_{\pm,u}|_{g=0}$ separately is a less trivial problem. For instance,

$$Z_{-,u}|_{g=0} = \mathrm{sp}\left(\exp(-\beta\Omega u^+ u) \sum_n \frac{(\beta t)^n}{n!} [\cos(\pi u^+ u)]^n \right)$$

$$= \mathrm{sp} \sum_n \exp(-\beta\Omega u^+ u) \frac{(\beta t)^n}{n!} \frac{1}{2^n} \sum_{m=0}^n C_n^m e^{i\pi(2m-n)u^+ u}$$

$$= \sum_n \frac{(\beta t)^n}{n!} \sum_{m=0}^n \frac{2^{-n} Z_v C_n^m}{1 - (-1)^{2m-n} e^{-\beta\Omega}} = \frac{\cosh \beta t}{1 - \exp(-\beta\Omega)} + \frac{\sinh \beta t}{1 + \exp(-\beta\Omega)}.$$

Similarly,

$$Z_{+,u}|_{g=0} = \frac{\cosh \beta t}{1 - \exp(-\beta\Omega)} - \frac{\sinh \beta t}{1 + \exp(-\beta\Omega)}$$

and therefore

$$Z|_{g=0} = Z_-|_{g=0} + Z_+|_{g=0} = \frac{2e^{\beta\mu} \cosh \beta t}{(1 - \exp(-\beta\Omega))^2}. \tag{11}$$

4. Low-temperature electron–phonon resonance for small hopping

We can construct the iterative procedure based upon the stationary phase approximation for the case when the electron-hopping integral is small: $t \ll \Omega, g$. It should be stressed that in our case the stationary phase approximation is valid only for large β (small temperature). It leads to equations on trajectories $\bar{u}, u$ with periodic boundary conditions $u(0) = u(\beta)$:

$$\dot{u} + \Omega u - \frac{g}{\sqrt{2}} \pm t(-2u)\exp[-2\bar{u}u] = 0$$
$$-\dot{\bar{u}} + \Omega\bar{u} - \frac{g}{\sqrt{2}} \pm t(-2\bar{u})\exp[-2\bar{u}u] = 0. \tag{12}$$

For small t the system of equations (12) has a solution which does not depend on the variable τ. The first approximation of this solution can be obtained via the general scheme [9] for the stationary phase approximation in the form

$$\bar{u}_0 = u_0 = \frac{g}{\sqrt{2}\,\Omega} \qquad \int D\bar{u}\, Du \, \exp S_{\pm,u} \simeq \frac{1}{\text{Det}\,\delta^2 S_{\pm,u}} \exp\{S_{\pm,u}|_0\}$$

where the kernel of the second variation of the action, for instance, $S_{-,u}$ is as follows:

$$\left.\frac{\delta^2 S_{-,u}}{\delta\bar{u}\,\delta u}\right|_0 = \left(\frac{\mathrm{d}}{\mathrm{d}\tau} + \Omega\right)\delta(\tau - \tau') + 2t\,(2\bar{u}u - 1)\exp(-2\bar{u}u).$$

Then the partition function takes the form

$$Z \cong \frac{e^{\beta\mu}\exp\left(g^2\beta/\Omega\right)}{1 - \exp(-\beta\Omega)}\left\{\frac{\exp[\beta t \exp(-g^2/\Omega^2)]}{1 - \exp(-\beta[\Omega - 2t\exp(-g^2/\Omega^2) + 2t(g^2/\Omega^2)\exp(-g^2/\Omega^2)])}\right.$$
$$\left. + \frac{\exp[-\beta t \exp(-g^2/\Omega^2)]}{1 - \exp(-\beta[\Omega + 2t\exp(-g^2/\Omega^2) - 2t(g^2/\Omega^2)\exp(-g^2/\Omega^2)])}\right\}. \tag{13}$$

We can see that for $\Omega = g \gg t$ the partition function (13) looks like

$$Z = e^{\beta(\Omega+\mu)}\frac{2\cosh(\beta t/e)}{(1 - e^{-\beta\Omega})^2}.$$

This formula represents the partition function of the system (1) without the electron–phonon interaction with the renormalization of parameters

$$\mu \to \mu + \Omega \qquad t \to \frac{t}{e}$$

of the initial electron energy and hopping. It means that the bound ('polaron'-type) electron–phonon state becomes unstable even for small hopping in the case of electron–phonon resonance.

As to the high-temperature asymptote for Z_u, we can obtain it via replacing the path integral with action (9) by a c-integral:

$$Z_{\pm,u} \sim \int \mathrm{d}\bar{u}\,\mathrm{d}u \, \exp\left[-\beta\left(\Omega\bar{u}u - \frac{g}{\sqrt{2}}(\bar{u} + u) \pm t\exp(-2\bar{u}u)\right)\right].$$

This integral can be represented as a t-series decomposition. It may be shown that the point $g = \Omega$ is not the point of resonance in this case, so at high temperature the electron–phonon decoupling for small hopping disappears.

5. Hopping renormalization for small electron–phonon interaction

In the case of small $g \ll t, \Omega$ we can estimate the partition function $Z_{\pm,u}$ in the following manner. The shift of the variables

$$w = u - \frac{g}{\sqrt{2}\,\Omega} \qquad \bar{w} = \bar{u} - \frac{g}{\sqrt{2}\,\Omega}$$

leads to the action

$$
\begin{aligned}
S_{\pm,u} &= -\int_0^\beta \left(\bar{w}\dot{w} + \Omega\bar{w}w \pm t \exp\left(-2\bar{w}w - \frac{\sqrt{2}\,g}{\Omega}(\bar{w}+w) - \frac{g^2}{\Omega^2} \right) - \frac{g^2}{2\Omega^2} \right) d\tau \\
&\approx \frac{\beta g^2}{2\Omega} - \int_0^\beta \left(\bar{w}\dot{w} + \Omega\bar{w}w \pm t\mathrm{e}^{(-g^2/\Omega^2)}\left(1 - \frac{\sqrt{2}g}{\Omega}(\bar{w}+w) + \frac{g^2}{\Omega^2}(\bar{w}+w)^2 \right)\mathrm{e}^{-2\bar{w}w} \right) d\tau.
\end{aligned}
$$
(14)

Now we use the iterative procedure and replace

$$(\bar{w}+w) \to \langle(\bar{w}+w)\rangle \qquad (\bar{w}+w)^2 \to \langle(\bar{w}+w)^2\rangle$$

where averages are taken from the $g = 0$ system. So,

$$\langle \bar{w} \rangle = \langle w \rangle = \langle \bar{w}^2 \rangle = \langle w^2 \rangle = 0$$

$$\langle \bar{w}w \rangle = \langle w\bar{w} \rangle = \bar{n} = -\frac{1}{\beta}\frac{\partial}{\partial\Omega} Z_{\pm,u}|_{g=0} = \mathrm{e}^{-\beta\Omega}\left\{ \frac{\cosh\beta t}{(1-\mathrm{e}^{-\beta\Omega})^2} \pm \frac{\sinh\beta t}{(1+\mathrm{e}^{-\beta\Omega})^2} \right\}.$$

Effectively we have the replacement

$$t_\pm \to t\exp\left[-\frac{g^2}{\Omega^2}\left(1 - 2\mathrm{e}^{-\beta\Omega}\left\{ \frac{\cosh\beta t}{(1-\mathrm{e}^{-\beta\Omega})^2} \pm \frac{\sinh\beta t}{(1+\mathrm{e}^{-\beta\Omega})^2} \right\} \right) \right]$$
(15)

and the partition function in this case looks like the one in (11) for $g = 0$ with renormalization of the hopping constant (15).

So, in the case of small electron–phonon interaction g we obtained the renormalization of the effective electron hopping (15). This renormalization is different for the symmetric and antisymmetric electron states.

6. Conclusion

We deduce the representation of the initial electron–phonon model (1) via two nonlinear phonon Hamiltonians H_- and H_+, corresponding to the symmetric and antisymmetric states of an electron. It means that we have calculated the partition function of the Holstein dimer with one electron over the electron variable. The derived phonon action contains a non-polynomial term, promoted by the electron hopping t. This calculation is, in some part, close to one performed in [10] for a Holstein dimer with two electrons; these authors used quantum-mechanical numerical calculations and investigated the ground state energy of the dimer, but not the partition function. In our paper the partition function over the phonon variables is represented via the coherent-state path integral. In spite of the complex form of the expressions obtained for the partition functions, remarkable consequences for special values of parameters of the system (1) may be seen. We analysed the special cases (sections 4 and 5) and obtained the effective description of the system in terms of non-interacting electron and phonons.

In the case of small-temperature, small-electron hopping $t \ll \Omega, g$, electron–phonon decoupling takes place as a consequence of the electron–phonon resonance condition $\Omega = g$.

The shift of the parameter μ and renormalization of the parameter t are similar to those obtained in polaron perturbation theory [2]. The resonance condition close to our condition $\Omega = g$ was obtained numerically in [11] for the response function of a two-level system, interacting with phonons.

In the case of a small electron–phonon interaction $g \ll t, \Omega$, when the polaron does not exist, we obtain renormalizations of the hopping constant t which are different for symmetric and antisymmetric electron states. We treat the case of a small difference between t_+ and t_- as testimony to the tendency for electron localization, as far as it denotes a large difference between the coefficients of the initial electron state.

We would like to touch on the problem of the transition to the trapping state which takes place in this type of two-level system. In our path-integral treatment the transition can be obtain as a branch point of the solution of the stationary phase approximation. One can easily see that the system (12) for small g has a single solution, and the second solution appears, as g increases. The same transition was investigated numerically for clusters [4, 7]. The localized states of the same type were shown numerically to appear instead of a band picture in the case of $g^2 \gg \Omega t$ in [12, 13]. This structure of the density of states was called in [12] 'resonances' in contrast to our term 'resonance' for the $\Omega = g$ case. Our low-temperature resonance $\Omega = g$ gives the condition when the tendency of a large polaron to transform to a small polaron for large $g > t$ is disturbed.

So, in our approach we eliminate the electron variable from the partition function of the Holstein dimer and derive the non-polynomial effective action for phonons. Such an approach happened to be suitable for an approximate analytical calculation that leads to a useful classification of electron–phonon statistical states.

Acknowledgments

Appendix

Let us obtain the explicit form of the permutation operator $\hat{P}_{\phi\psi}$. Based upon the corresponding term in the action, we try to construct a permutation operator of the form

$$\hat{P}_{\phi\psi} = \exp(\alpha\phi^+\psi + \beta\psi^+\phi)\exp(\gamma\phi^+\phi + \delta\psi^+\psi).$$

The equalities

$$\exp(\alpha\phi^+\psi + \beta\psi^+\phi)\phi^+\exp(-\alpha\phi^+\psi - \beta\psi^+\phi) = \phi^+\cosh\sqrt{\alpha\beta} + \psi^+\sqrt{\frac{\beta}{\alpha}}\sinh\sqrt{\alpha\beta}$$

$$\exp(\alpha\phi^+\psi + \beta\psi^+\phi)\psi^+\exp(-\alpha\phi^+\psi - \beta\psi^+\phi) = \psi^+\cosh\sqrt{\alpha\beta} + \phi^+\sqrt{\frac{\beta}{\alpha}}\sinh\sqrt{\alpha\beta}$$

and

$$\exp(\gamma\phi^+\phi + \delta\psi^+\psi)\phi^+\exp(-\gamma\phi^+\phi - \delta\psi^+\psi) = \exp(\gamma)\phi^+$$

$$\exp(\gamma\phi^+\phi + \delta\psi^+\psi)\psi^+\exp(-\gamma\phi^+\phi - \delta\psi^+\psi) = \exp(\delta)\psi^+$$

show, that we should choose $\sqrt{\alpha\beta} = i\pi/2$, $\exp(-\delta) = \sqrt{\beta/\alpha}\sinh\sqrt{\alpha\beta}$ and $\exp(-\gamma) = \sqrt{\alpha/\beta}\sinh\sqrt{\alpha\beta}$. It is enough to choose $\alpha = \beta = i\pi/2$, $\gamma = \delta = -i\pi/2$. The other solution

is as follows: $\alpha = \beta = -i\pi/2$, $\gamma = \delta = i\pi/2$. So, we can choose the Hermitian form of the permutation operator:

$$\hat{P}_{\phi\psi} = \cos\left[\tfrac{1}{2}\pi(-\phi^+\phi - \psi^+\psi + \phi^+\psi + \psi^+\phi)\right].$$

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