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Stability of a bipolaron in a one-dimensional system coupled with dopants

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Abstract. The stability of a bipolaron is examined in a single polymer chain coupled with dopants considering up to the nearest-neighbour site diagonal electron–phonon (e–p) interactions. The behaviour of the bipolaron depending on the e–p coupling constant and the on-site Coulomb repulsion is studied within the framework of unrestricted Hartree–Fock theory using an extended Lang–Firsov transformation and a squeeze transformation. It is shown that dopants play an important role in the stabilization of the bipolaron and, moreover, that this stability appears under subtle conditions. In particular, the bipolaron separates into two polarons by the smaller on-site Coulomb interaction in the strong e–p coupling regime.

1. Introduction

Various non-linear excitations in the quasi-one-dimensional (Q-1D) system have been discussed with the use of simplified 1D models, from which many fruitful results have been obtained. In particular, *trans*-polyacetylene (*t*-PA), a system with a degenerate ground-state structure, is accompanied by soliton excitations in the non-doped state [1]. Within the approximation of the Su–Schrieffer–Heeger (SSH) [2] or Takayama–Lin–Liu–Maki [3] Hamiltonian, this type of excitation has been successfully investigated by many researchers. After doping in *t*-PA, the neutral solitons with one-half spin change into spinless charged solitons, with an electrical conductivity increase [1].

On the other hand, it is well known that some conducting polymers such as poly(*p*-phenylene) and polythiophene also show spinless transport [1]. This means that the characteristic soliton model for *t*-PA is not applicable to such conducting polymers because these polymers do not possess a degenerate ground state. As a result, it has been rather ambiguously thought that a plausible explanation for the spinless transport of this kind of polymer has been given in terms of the bipolaron-transport model [1]. Here, we use the word ‘bipolaron’ in the sense of a small bipolaron arising as the consequence of the competition of the Coulomb repulsion and the self-trapping net attraction between two polarons [4]. This is a rather tough entity to treat theoretically. Therefore, not many attempts have been made with respect to the problem of theoretical explanations about the stability of bipolarons in conducting polymers [5–11].

The problem of interchain stability, namely transverse transfer of polarons in conductive polymers, has caused a great deal of controversy. Over the past few years, it has been suggested that some disorder effects such as defects or impurities can stabilize the polaron and bipolaron in actual conductive polymers [12–15]. Hence, it is of interest to check how

defects and impurities can influence the stability and structure of the polaron and bipolaron. As for the effect of defects in polymer chains, Mizes and Conwell [16] have recently shown in a two-chain discrete SSH model that chain endings and conjugation breaks can stabilize the polaron and bipolaron. The effect of a dopant on the interchain stability of polaronic excitation in conducting polymers has been examined in both continuum [12, 14] and discrete models [15] on the basis of the Holstein Hamiltonian. However, the role of dopant, which is the most important impurity in conducting polymers, has been somewhat disregarded in the theoretical discussion of the interchain stability of bipolarons.

In the present study, we investigate the influence of dopants on a bipolaron generated in a single polymer chain, as the first step to obtaining a clear understanding of the mechanism of interchain transport of bipolarons assisted by dopants. For this purpose, we adopt a simple model Hamiltonian including up to nearest-neighbour site diagonal electron–phonon (e–p) interactions for a single polymer chain coupled with dopants.

2. Theoretical analysis

The model Hamiltonian for a single chain coupled with dopants is a modification of the standard Holstein [17] Hamiltonian to describe electrons locally coupled to molecular-like oscillators. The Hamiltonian in the present work has a more explicit form ($\hbar = 1$):

$$\begin{aligned}
 H = & -t_{\parallel} \sum_{i,\sigma} (c_{i+1,\sigma}^{\dagger} c_{i,\sigma} + c_{i,\sigma}^{\dagger} c_{i+1,\sigma}) + U \sum_i n_{i,\alpha} n_{i,\beta} + \omega \sum_i b_i^{\dagger} b_i + g_1 \sum_{i,\sigma} n_{i,\sigma} (b_i + b_i^{\dagger}) \\
 & + g_2 \sum_{i,\sigma} \sum_{\delta} n_{i,\sigma} (b_{i+\delta} + b_{i+\delta}^{\dagger}) - t_D \sum_{i,\sigma} (c_{D_i,\sigma}^{\dagger} c_{d_i,\sigma} + c_{d_i,\sigma}^{\dagger} c_{D_i,\sigma}) \\
 & + U' \sum_i n_{D_i,\alpha} n_{D_i,\beta} + \omega' \sum_i b_{D_i}^{\dagger} b_{D_i} + g'_1 \sum_{i,\sigma} n_{D_i,\sigma} (b_{D_i} + b_{D_i}^{\dagger}) \\
 & + g'_2 \sum_{i,\sigma} n_{D_i,\sigma} (b_{d_i} + b_{d_i}^{\dagger}) \quad n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma} \quad (1)
 \end{aligned}$$

where $c_{i,\sigma}^{\dagger}$ ($c_{i,\sigma}$) is the creation (annihilation) operator of the electron at the i th site with spin σ ($= \alpha, \beta$), b_i^{\dagger} (b_i) is the creation (annihilation) operator of the phonon at the i th site, which is assumed to be dispersionless for simplicity, and ω (ω' for dopant sites) represents the frequency of the phonon subsystem. As shown in figure 1, D_i denotes a dopant site with $i = 1 \sim N_D$. The site d_i in the polymer chain stands for the nearest-neighbour site to the dopant site D_i . This Hamiltonian includes the intersite-transfer part of the electron in the unperturbed chain with transfer integral t_{\parallel} , the transfer part from the site d_i to the dopant site D_i with t_D , the on-site Coulomb repulsion U (U' on the dopant sites) between electrons of different spins, and the site-diagonal e–p interaction with coupling constant g_1 (g'_1 for the dopant sites). Moreover, the nearest-neighbour site-diagonal e–p interaction with coupling constant g_2 (g'_2 for the dopant sites) is introduced into the Hamiltonian to treat more wide-ranging lattice deformations around the electron. In the presence of such deformation-type e–p interaction, the modulation of the on-site energy is caused by the extended lattice deformation. The summation over δ represents that over the nearest-neighbour sites.

Applying a unitary transformation of the extended Lang–Firsov [18] type [19] according

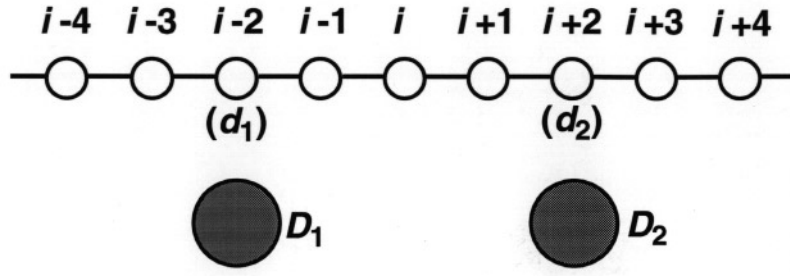


Figure 1. Schematic drawing of the present model system where two dopants couple with a single polymer chain.

to

$$S = \exp R$$

$$R = \sum_{i,\sigma} \left(\frac{g_1}{\omega} n_{i,\sigma} (b_i^\dagger - b_i) + \frac{g_2}{\omega} \sum_{\delta} n_{i,\sigma} (b_{i+\delta}^\dagger - b_{i+\delta}) \right) + \sum_{i,\sigma} \left(\frac{g'_1}{\omega'} n_{D_i,\sigma} (b_{D_i}^\dagger - b_{D_i}) + \frac{g'_2}{\omega'} n_{D_i,\sigma} (b_{d_i}^\dagger - b_{d_i}) \right) \quad (2)$$

and taking the average of the transformed Hamiltonian over the phonon-vacuum state $|0\rangle$, we have the following effective Hamiltonian H_{eff} :

$$H_{eff} = \langle 0 | S H S^\dagger | 0 \rangle = -t_{\parallel} \sum_{i,\sigma} (c_{i+1,\sigma}^\dagger c_{i,\sigma} + c_{i,\sigma}^\dagger c_{i+1,\sigma}) \exp(-f_i) + \sum_i U_{eff}^i n_{i,\alpha} n_{i,\beta} + \sum_{i,\sigma} \varepsilon_P^i n_{i,\sigma} + V_1 \sum_{i,\sigma,\sigma'} n_{i,\sigma} n_{i+1,\sigma'} + V_2 \sum_{i,\sigma,\sigma'} n_{i,\sigma} n_{i+2,\sigma'} + N\omega - t_D \sum_{i,\sigma} (c_{D_i,\sigma}^\dagger c_{d_i,\sigma} + c_{d_i,\sigma}^\dagger c_{D_i,\sigma}) \exp(-f') + U'_{eff} \sum_i n_{D_i,\alpha} n_{D_i,\beta} + \varepsilon'_P \sum_{i,\sigma} n_{D_i,\sigma} + W_1 \sum_{i,\sigma,\sigma'} n_{D_i,\sigma} n_{d_i,\sigma'} + W_2 \sum_{i,\sigma,\sigma'} \sum_{\delta} n_{D_i,\sigma} n_{d_{i+\delta},\sigma'} + N_D \omega' \quad (3)$$

where N is the total number of sites in the polymer chain. The representations of the other parameters in equation (3) are given in appendix. It should be noted that V_1 , V_2 , W_1 and W_2 (equations (A7)–(A10)) have negative values, which means that the attractive interaction occurs between two electrons.

Since we are going to study a negative bipolaron on a single chain, we assume that there are $N + 2$ electrons in the chain. For the numerical analysis, we use the unrestricted Hartree–Fock scheme, i.e. ‘the different orbital for the different spin’ scheme. Let $\varepsilon_{k,\sigma}$ and $\psi_{k,\sigma}$ be the eigenvalues and eigenfunctions of H_{eff} , respectively and $c_i^{(k,\sigma)}$ the coefficient of the π orbital centred on the i th site in the linear combination of atomic orbitals expansion of $\psi_{k,\sigma}$. The coefficient $c_i^{(k,\sigma)}$ satisfies the following equation:

$$\varepsilon_{k,\sigma} c_i^{(k,\sigma)} = [\varepsilon_P^i + V_1 \{ \langle n_{i-1} \rangle + \langle n_{i+1} \rangle \} + V_2 \{ \langle n_{i-2} \rangle + \langle n_{i+2} \rangle \} + U_{eff}^i \langle n_{i,-\sigma} \rangle] c_i^{(k,\sigma)} + (-t_{\parallel} \exp(-f_i) - V_1 m_{i,\sigma}) c_{i+1}^{(k,\sigma)} + (-t_{\parallel} \exp(-f_i) - V_1 m_{i-1,\sigma}) c_{i-1}^{(k,\sigma)} - V_2 m'_{i,\sigma} c_{i+2}^{(k,\sigma)} - V_2 m'_{i-2,\sigma} c_{i-2}^{(k,\sigma)} + W_1 \langle n_{D_i} \rangle c_{d_i}^{(k,\sigma)} + W_2 \langle n_{D_i} \rangle c_{d_{i\pm 1}}^{(k,\sigma)} \quad (4)$$

$$\langle n_i \rangle = \langle n_{i,\alpha} \rangle + \langle n_{i,\beta} \rangle$$

where $\langle n_{i,\sigma} \rangle$, $m_{i,\sigma}$ and $m'_{i,\sigma}$ are the averages of $n_{i,\sigma}$, $c_{i+1,\sigma}^\dagger c_{i,\sigma}$ and $c_{i+2,\sigma}^\dagger c_{i,\sigma}$, respectively. These should be determined self-consistently.

In equation (4), we assume that $\langle n_{D_i,\alpha} \rangle = \langle n_{D_i,\beta} \rangle = 0.5$. This assumption corresponds to neglecting fluctuation of the electron density over the dopants. On the basis of these, we investigate the stability of the bipolaron due to the additional lattice deformation induced by dopants. Furthermore, to avoid the end effect [20], we impose the Born–von Kármán boundary condition on a 100-site chain.

3. Results and discussion

The parameters used are $t_{\parallel} = 2.0$ eV (a plausible value for conducting polymers [1]), $U = 1.0$ eV and $\omega (= \omega') = 0.2$ eV. This ω nearly equals the frequency of the stretching mode of the carbon–carbon double bond. No experimental estimation of g_1 , g_2 , g'_1 and g'_2 for conducting polymers is available to the best of our knowledge. Hence, we assume that $g_1 = 0.2$ eV and $g_2 = 0.05$ eV in the intermediate-coupling regime. The modified Lang–Firsov transformation leads to the so-called self-trapped state in the strong e–p interaction regime as examined by Das and Sil [19]. We observed non-convergence in calculating the regime such that $g_1/\omega > 2$, indicating self-trapping. However, the present analysis is effective for arbitrary parameters in the range $g_1/\omega < 2$ frequently applied to conductive polymers such as polyacetylene [13]. In the region $g_1/\omega < 2$, the calculations generally converged within several self-consistent field cycles.

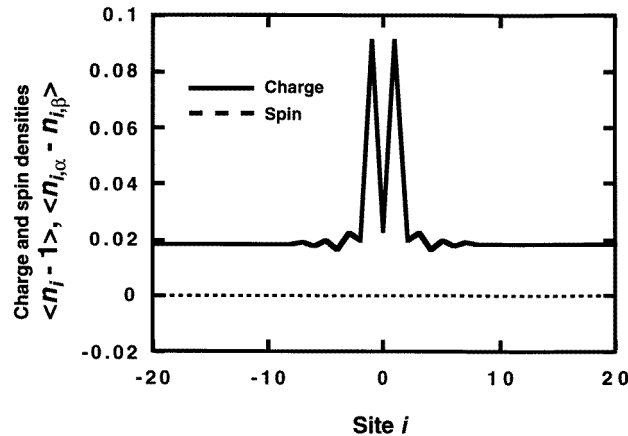


Figure 2. Charge- and spin-density profiles of a bipolaron with $l_D = 2$, $t_{\parallel} = 2.0$, $U = 1.0$, $g_1 = g'_1 = 0.2$ and $g_2 = g'_2 = 0.05$ (in electronvolts except l_D).

For these appropriate parameters, the charge and spin densities are obtained as seen in figure 2. What has to be noted is that the spin density becomes zero at all the sites, signifying that this bipolaron is a singlet. Once such a singlet bipolaron is formed, the system shows non-magnetic properties, while the electric conductivity is not changed. However, it should be emphasized that, when the dopants are removed from the system, the ground state is the charge density wave (CDW) state, delocalized all over the sites unlike that in figure 2. In other words, the system reveals the bipolaron only after the doping. This bipolaron can be regarded as a weakly localized entity formed and bound by the dopants rather than as a mobile entity. Furthermore, it is seen that the bipolaron is more stabilized on increasing

the number of dopants; a one-dopant system is stabilized by 0.153 eV and a two-dopant system by 0.312 eV, compared with the total energy of the dopant-free system.

The stability of the bipolaron was examined for various values of the interdopant distance l_D (in units of the lattice constant). A local energy minimum of the bipolaron was found at around $l_D = 2$, which is only stable by 10^{-3} eV compared with other values of l_D . Usually, the artificial lattice deformation consisting of the tangent hyperbolic function has been introduced in phonon subsystem [1]. Thus an energetically stable polaron (or bipolaron) can be formed. In contrast, this shallow potential obtained in the present work is probably derived from taking the average of SHS^\dagger over the phonon vacuum state in order to obtain equation (3). Nevertheless, our methodology succeeded in describing some aspects of the bipolaron such as the separation into two polarons and so forth, due to incorporation of the dopants.

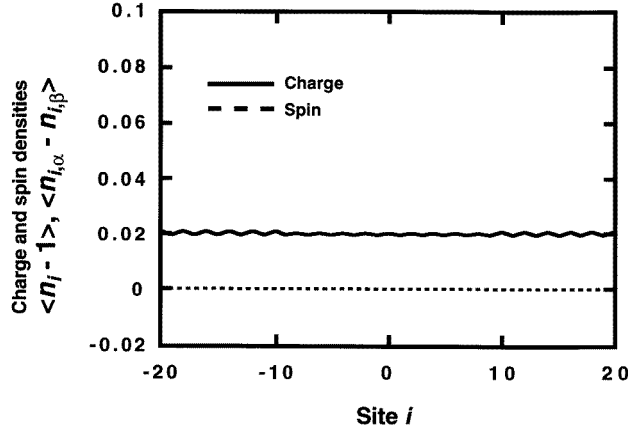


Figure 3. Charge- and spin-density profiles for $l_D = 2$, $t_{\parallel} = 2.0$, $U = 1.0$, $g_1 = g'_1 = 0.2$ and $g_2 = g'_2 = 0$ (in electronvolts except l_D).

Next, setting $g_2(=g'_2) = 0$, we found that the charge density delocalizes over all the sites as shown in figure 3. It is thus apparent that the nearest-neighbour site-diagonal e–p interaction affects the formation of bipolaron, even though the coupling constant is not so large. Moreover, we calculated for smaller values of g'_1 and g'_2 than those of g_1 and g_2 , in order to confirm whether the bipolaron scheme is changed or not. This is because the vibration between the polymer chain and the dopant molecule is weaker than the intersite vibration. However, it is verified that the tendency of the charge distribution does not change.

The role of the electron–electron correlations, particularly the on-site Coulomb type, becomes crucial in the bipolaron stability, since the charge of singlet bipolaron tends to concentrate in the vicinity of the dopants according to the increase in the e–p interaction. In figure 4, we show the charge and spin densities for the system with strong e–p coupling ($g_1/\omega = 2$). It is seen that the positive and the negative spins appear in the vicinity of the dopants, signifying the separation of the bipolaron into two polarons even for the smaller value of U (> 1). Also, it is clearly seen that such strong e–p interaction leads to the CDW. The results suggest that

(i) the bipolaron can only exist in a delicate balance among the parameters t_{\parallel} , U , g_1 and g_2 and, in particular, in the strong e–p coupling regime and

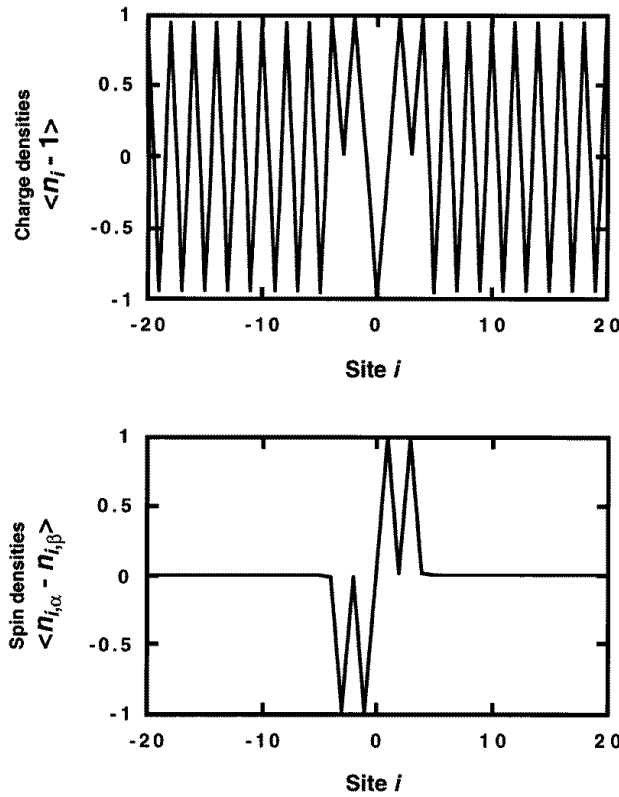


Figure 4. Charge- and spin-density profiles for $l_D = 2$, $t_{\parallel} = 2.0$, $U = 1.0$, $g_1 = g'_1 = 0.4$ and $g_2 = g'_2 = 0.01$ (in electronvolts except l_D).

(ii) the nearest-neighbour site-diagonal e–p interaction and the on-site Coulomb repulsion terms are necessary for a more realistic calculation.

Let us consider here another effective Hamiltonian. In polaron theory, a unitary transformation such as equation (2) is conventionally applied to the Hamiltonian H , so that the well known Holstein [17] reduction factor such as equation (4) can be obtained after averaging SHS^\dagger over the vacuum state of phonon subsystem. This factor leads to the self-trapping of the polaron in the strong e–p interaction regime. Recently, Zheng [21] has shown, however, that the ordinary polaronic state must be replaced by the squeezed polaronic state so as to find a new and more energetically stable state. In this squeezed state, the phonon subsystem is transformed into the two-phonon coherent state [22] by introducing a variational ground state $|\alpha\rangle$ for the phonon subsystem in order to lower the total energy:

$$\begin{aligned}
 |\alpha\rangle &= \exp(-R)|0\rangle \\
 R &= \sum_i \alpha(b_i b_i - b_i^\dagger b_i^\dagger)
 \end{aligned}
 \tag{5}$$

where α is a variational parameter.

Averaging SHS^\dagger over the variational ground state $|\alpha\rangle$, a new effective Hamiltonian, in which $\exp(-f_i)$ and ω in equation (3) are replaced by $\exp(-f_i \exp(-4\alpha))$ and $\omega[\sinh(2\alpha)]^2$, respectively, is obtained. The relative energy per site is plotted for different values of α in

figure 5. The parameters used are the same as those in figure 2. The squeezed polaronic state leads to a net-energy gain, because the Holstein reduction factor is weakened while the strong e-p interaction is maintained. Therefore, the squeeze transformation of equation (5) must be important for examining the system in the strong e-p interaction regime. When $\alpha = 0.42$, the charge and spin are delocalized extensively compared with the case $\alpha = 0$. This means that, by applying the squeeze transformation, relaxation of the highly distorted lattice apparently leads to an increase in the transfer integral t_{\parallel} . Without the squeeze transformation, we observed oscillatory non-convergent behaviours in calculating the strong e-p coupling regime. However, this situation is obviated by the transformation probably due to the above-mentioned improvement in t_{\parallel} .

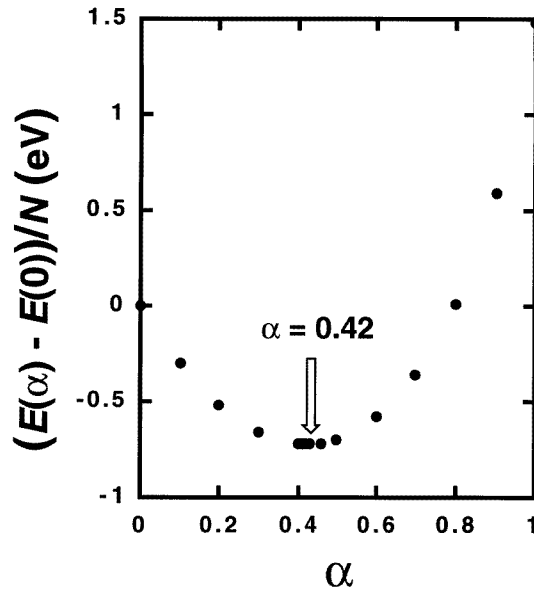


Figure 5. $(E(\alpha) - E(0))/N$ versus α plots under $I_D = 2$, $t_{\parallel} = 2.0$, $U = 1.0$, $g_1 = g'_1 = 0.2$ and $g_2 = g'_2 = 0.05$ (in electronvolts except I_D). The arrow indicates the optimized value for the variational parameter $\alpha = 0.42$.

We conclude that the bipolaron can be stabilized in the presence of dopants, which bring a new lattice structure into Q-1D solids. This, of course, it is possible only under suitable conditions, from which the bipolaron decomposes into two polarons. In particular, the bipolaron separates into two polarons by the smaller on-site Coulomb interaction in the strong e-p coupling regime. The analysis of the system containing two or more chains coupled with dopants is required to illuminate the mechanism of the dopant-assisted bipolaron transverse conduction in conductive polymers. We believe that this issue will be effectively and visually described by the present method and will be reported elsewhere.

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Appendix

Here we represent the parameters in equation (3):

$$f_i = \begin{cases} \frac{g_1^2}{\omega^2} - 2\frac{g_1g_2}{\omega^2} + 3\frac{g_2^2}{\omega^2} & \text{(when both } i \text{ and } i+1 \text{ are the nearest-neighbouring} \\ & \text{sites to dopants)} \\ \frac{g_1^2}{\omega^2} - 2\frac{g_1g_2}{\omega^2} + \frac{5g_2^2}{2\omega^2} & \text{(when either } i \text{ or } i+1 \text{ is the nearest-neighbour site} \\ & \text{to a dopant)} \\ \frac{g_1^2}{\omega^2} - 2\frac{g_1g_2}{\omega^2} + 2\frac{g_2^2}{\omega^2} & \text{(elsewhere)} \end{cases} \quad (\text{A1})$$

$$f' = \frac{1}{2} \left(\frac{g_1'}{\omega'} - \frac{g_2}{\omega} \right)^2 + \frac{1}{2} \left(\frac{g_1}{\omega} - \frac{g_2'}{\omega'} \right)^2 + \frac{g_2^2}{\omega^2} \quad (\text{A2})$$

$$U_{eff}^i = \begin{cases} U - 2\frac{g_1^2}{\omega} - 4\frac{g_2^2}{\omega} + 2\frac{g_2'^2}{\omega'} & \text{(for } i = d_i) \\ U - 2\frac{g_1^2}{\omega} - 4\frac{g_2^2}{\omega} & \text{(elsewhere)} \end{cases} \quad (\text{A3})$$

$$U'_{eff} = U' - 2\frac{g_1'^2}{\omega'} - 4\frac{g_2'^2}{\omega'} + 2\frac{g_2^2}{\omega} \quad (\text{A4})$$

$$\varepsilon'_p = \begin{cases} -\frac{g_1^2}{\omega} - 2\frac{g_2^2}{\omega} + \frac{g_2'^2}{\omega'} & \text{(for } i = d_i) \\ -\frac{g_1^2}{\omega} - 2\frac{g_2^2}{\omega} & \text{(elsewhere)} \end{cases} \quad (\text{A5})$$

$$\varepsilon'_p = -\frac{g_1'^2}{\omega'} - 2\frac{g_2'^2}{\omega'} + \frac{g_2^2}{\omega} \quad (\text{A6})$$

$$V_1 = -\frac{4g_1g_2}{\omega} \quad (\text{A7})$$

$$V_2 = -\frac{2g_2^2}{\omega} \quad (\text{A8})$$

$$W_1 = -\frac{2g_1g_2}{\omega} - \frac{2g_1'g_2'}{\omega'} \quad (\text{A9})$$

$$W_2 = -\frac{2g_2'^2}{\omega'}. \quad (\text{A10})$$

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