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Local density of states of dc-biased superlattices with time-dependent imperfection*

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The single-particle Green's function for a dc-biased superlattices with single impurity potential varying harmonically with time has been obtained in the framework of $U(t,t')$ method and Floquet–Green's function. The calculation of the local density of states shows that new states will emerge between the resonant Wannier–Stark states as a result of the intervention of time-dependent impurity potential, and the increase in electric field strength of impurity will result in the growing of the number of new states between the gaps of neighbouring Stark ladders.

Keywords: local density of states, Floquet-Green's function, defects and impurity
PACC: 7120A, 7210F, 7115P

1. Introduction

Quantum electronic transport properties in semiconductor superlattices under the influence of electric fields have been a much interesting subject of research in recent years. The well-known controversial physical phenomena, Bloch oscillations and Wannier–Stark ladders in a dc-biased crystal solids, have been verified in superlattices by various experimental groups.[1−3] Moreover, many novel and interesting theoretical predictions and experimental findings have been reported in electric-field biased superlattices, among these, the typical ones are negative differential conductivity,[4] dynamical localization,[5] and fractional Wannier–Stark ladder driven by dc and ac electric fields,[6] band suppression[7] and Shapiro effect.[8]

There are many ways of treating the problems of the superlattices driven by an external electric field, which are essentially nonequilibrium phenomena. The common way is to utilize the time-dependent Schödinger equation,

$$\left[\mathcal{H}(x) - \mathrm{i}\frac{\partial}{\partial t}\right]\psi(x,t) = 0, \tag{1}$$

where $\mathcal{H}(x)$ is the crystal Hamiltonian plus the external potential induced by electric fields. Particularly, if the external electric fields are time-periodic with a period of T, Floquet theorem can be employed:[6]

$$\left[\mathcal{H}(x,t) - \mathrm{i}\frac{\partial}{\partial t}\right]u_\epsilon(x,t) = \epsilon u_\epsilon(x,t), \tag{2}$$

where $u_\epsilon(x,t) = \exp(\mathrm{i}\epsilon t)\psi(x,t)$, and $u_\epsilon(x,T) = u_\epsilon(x,0)$. Using these equations, dynamical quantities such as mean-square displacement, electric currents etc can be obtained.[5,9,10]

Another important approach is implemented through the use of the single-particle Green's function from which dynamical properties can be drawn out.[11,12] The typical example is density of states which can be obtained from the imaginary part of spectral function,

$$n(E) = \frac{1}{2\pi}\mathrm{Tr}\ A(E), \tag{3}$$

while the spectral function is closely related to the retarded Green's function through the following relation:

$$\begin{aligned} G^r(x,t;x',t') &= -\mathrm{i}\theta(t-t')\langle\{\Psi(x,t),\Psi^\dagger(x't')\}\rangle \\ &= -\mathrm{i}\theta(t-t')A(x,t;x't'). \end{aligned} \tag{4}$$

By choosing a gauge-invariant spectral function,[13] density of states can be obtained straightforwardly.

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More recently, a method called Floquet–Green's function[14] has been developed to calculate dynamical properties of a general time-periodic Hamiltonian. This method is essentially the $U(t,t')$ method, previously invented by Moiseyev group.[15] The essential mathematics behind this method lies in that the genuine time variable involved in the original Hamiltonian is treated as a spatial variable, while a new pseudo-time variable is introduced. This method will be explained in detail in Section 3 of this paper.

In Section 2, we use the single-particle Green's function formalism to calculate the site-diagonal element of Green's function of a tight-binding model driven by an external uniform electric field, through which the local density of states can be derived. In Section 3, the dc electric field-biased tight-binding Hamiltonian with a defect energy harmonically changing with time is investigated. The analytical continued fraction expression for local density of states is obtained. Through this analytical expression, further numerical computation is given to study the influence of the time-periodically varying impurity on the structure of local density of states by adjusting the different parameters involved in the system.

2. Site-diagonal Green's function of a dc-biased tight-binding model

Considering a superlattices under the influence of a uniform dc-electric field, the corresponding Hamiltonian can be described in terms of tight-binding approximation for simplicity as follows:

$$\begin{aligned}\mathcal{H}_{\mathrm{TB}} =& t\sum_n \left(|n+1\rangle\langle n| + |n\rangle\langle n+1|\right) \\ &+ \sum_n neFd\,|n\rangle\langle n|\,, \end{aligned} \tag{5}$$

where $|n\rangle$ is the localized Wannier basis, t is the hopping term characterizing the energy band width in the absence of the external field, F being the external uniform electric field, d being the superlattice constant, and $-e$ being the electron charge.

If the quantity $neFd$ in the last term on the right-hand side of the above equation is regarded as V_n, then Green's function formalism exhaustively explicated in Ref.[16] can be employed to derive the single-particle Green's function $G(n,n;\epsilon)$ as follows:

$$G(n,n;\epsilon) = \cfrac{1}{\epsilon - V_n - \cfrac{t^2}{\epsilon - V_{n+1} - \cfrac{t^2}{\epsilon - V_{n+2} - \cfrac{t^2}{\vdots}}} - \cfrac{t^2}{\epsilon - V_{n-1} - \cfrac{t^2}{\epsilon - V_{n-2} - \cfrac{t^2}{\vdots}}}}, \tag{6}$$

where ϵ is the complex-valued energy variable.

For simplicity, we focus on the Green's function at site zero $G(0,0;\epsilon)$. Inverting Eq.(6), and denoting $\alpha \equiv eFd$, the following relation can be obtained:

$$\begin{aligned} G_{00}^{-1}(\epsilon) =& \epsilon - \cfrac{t^2}{\epsilon - \alpha - \cfrac{t^2}{\epsilon - 2\alpha - \cfrac{t^2}{\vdots}}} \\ &- \cfrac{t^2}{\epsilon + \alpha - \cfrac{t^2}{\epsilon + 2\alpha - \cfrac{t^2}{\vdots}}}. \end{aligned} \tag{7}$$

By invoking the following identity associated with the first-kind of Bessel functions,

$$\frac{y}{2\nu}\frac{J_{\nu-1}(y)}{J_\nu(y)} - 1 = \cfrac{-\cfrac{\left(\frac{y}{2}\right)^2}{\nu(\nu+1)}}{1 - \cfrac{\left(\frac{y}{2}\right)^2}{(\nu+1)(\nu+2)}}, \tag{8}$$

the last two terms on the right-hand side of Eq.(7) can be simplified after a tedious algebra into the following form:

$$G_{00}^{-1}(\epsilon) = \frac{\epsilon y}{2\nu}\frac{J_{\nu-1}(y)}{J_\nu(y)} - \frac{\epsilon y}{2\nu}\frac{J_{-\nu-1}(y)}{J_{-\nu}(y)} - \epsilon, \tag{9}$$

where $\nu = \dfrac{\epsilon}{\alpha}$, and $y = \dfrac{2t}{\alpha}$.

Using the following iterative relationships among

the first-kind Bessel functions:

$$J_{\nu+1}(y)J_{-\nu}(y)+J_{-\nu-1}(y)J_{\nu}(y)=\frac{-2\sin(\nu\pi)}{\pi y}, \tag{10a}$$

$$J_{\nu-1}(y)+J_{\nu+1}(y)=\frac{2\nu}{y}J_{\nu}(y), \tag{10b}$$

Equation (9) can be simplified into the following form:

$$G_{00}^{-1}(\epsilon)\equiv\frac{\alpha}{\pi}\frac{\sin\left(\frac{\epsilon}{\alpha}\pi\right)}{J_{\frac{\epsilon}{\alpha}}\left(\frac{2t}{\alpha}\right)J_{-\frac{\epsilon}{\alpha}}\left(\frac{2t}{\alpha}\right)}. \tag{11}$$

When $1/\alpha\to\infty$, we use the asymptotic Bessel functions

$$\lim_{y\to\infty}J_{\pm\nu}(y)=\sqrt{\frac{2}{\pi y}}\cos\left(y\mp\frac{1}{2}\nu\pi-\frac{1}{4}\pi\right), \tag{12}$$

and we obtain after some algebraic manipulations that

$$a(\epsilon)=2t\left(\frac{\sin(\frac{\epsilon}{\alpha}\pi)}{\sin(\frac{4t}{\alpha})+\cos(\frac{\epsilon}{\alpha}\pi)}\right). \tag{13}$$

3. Local density of states of dc-biased tight-binding model with time-harmonically varying impurity

In the previous section, the Green's function for a tight-binding model driven by a uniform dc electric field can be obtained directly from Eq.(6) in a standard way,[17] which however does not hold true if time-dependent electric field is involved in the system. In fact, Moiseyev and co-workers have developed a similar method to tackle the problem, which is so-called $U(t,t')$ method. As pointed out in the Introduction of this paper, by treating time- and space-variables on the same footing, Floquet Hamiltonian can be defined as follows:

$$\mathcal{H}^{\mathrm{F}}(x,t')=\mathcal{H}(x,t')-\mathrm{i}\hbar\frac{\partial}{\partial t'}. \tag{14}$$

The Green's function corresponding to Hamiltonian $H^{\mathrm{F}}(x,t')$ can be written in a similar way to that for the time-independent case[18] as follows:

$$\begin{aligned}&G^{\mathrm{F}}(\epsilon|x,x',t't'')\\&=\int\mathrm{d}\epsilon'\sum_n\frac{\psi_n^*(\epsilon|x,t')\psi_n(\epsilon'|x',t'')}{\epsilon-\epsilon'},\end{aligned} \tag{15}$$

where wavefunctions $\psi_n^*(\epsilon'|x,t)$ constitute a complete set of eigenfunctions corresponding to the operator $H^{\mathrm{F}}(x,t)$. The above Floquet–Green's function satisfies the following inhomogeneous equations similar to those for a time-independent case[14]

$$\begin{aligned}&\left[\epsilon-\mathcal{H}^{\mathrm{F}}(x,t')\right]G^{\mathrm{F}}(\epsilon|x,x';t't'')\\&=\delta(x-x')\delta(t-t').\end{aligned} \tag{16}$$

Due to the time-periodicity of $\psi_n^*(\epsilon'|x,t)$ over t, Eq.(16) can be Fourier transformed into the following form in spectrum space

$$\begin{aligned}&\epsilon G^{\mathrm{F}}_{\alpha,\beta}(x,x')-\mathcal{H}^{\mathrm{F}}_{\alpha,\gamma}(x)G^{\mathrm{F}}_{\gamma,\beta}(\epsilon|x,x')\\&=\delta(x-x')\delta_{\alpha,\beta},\end{aligned} \tag{17}$$

where summation over repeated indices is always understood. Once the above matrix form is established, the Green's function for a harmonically driven Hamiltonian $\mathcal{H}=\mathcal{H}_0+\mathcal{V}_0+2\mathcal{V}_1\cos(\omega t')$ can be obtained through the introduction of effective potential $\mathcal{V}_{\mathrm{eff}}(E)$ and straightforward algebra as follows:[14]

$$g^{\mathrm{D}}(E)=\frac{1}{[E-(\mathcal{H}_0+\mathcal{V}_0)-\mathcal{V}_{\mathrm{eff}}(E)]}, \tag{18}$$

where

$$\mathcal{V}_{\mathrm{eff}}(E_\beta)=\mathcal{V}^{\uparrow}_{\mathrm{eff}}(E_\beta)+\mathcal{V}^{\downarrow}_{\mathrm{eff}}(E_\beta), \tag{19a}$$

$$\mathcal{V}^{\uparrow}_{\mathrm{eff}}(E_\beta)=\mathcal{V}_1\cfrac{1}{C_{\beta+1}-\mathcal{V}_1\cfrac{1}{C_{\beta+2}-\mathcal{V}_1\cfrac{1}{\vdots}\mathcal{V}_1}\mathcal{V}_1}\mathcal{V}_1, \tag{19b}$$

$$\mathcal{V}^{\downarrow}_{\mathrm{eff}}(E_\beta)=\mathcal{V}_1\cfrac{1}{C_{\beta-1}-\mathcal{V}_1\cfrac{1}{C_{\beta-2}-\mathcal{V}_1\cfrac{1}{\vdots}\mathcal{V}_1}\mathcal{V}_1}\mathcal{V}_1, \tag{19c}$$

$$\begin{aligned}C_\beta&=E_\beta+\beta\hbar\omega-(\mathcal{H}_0+\mathcal{V}_0)\\&\equiv\epsilon+\beta\hbar\omega-(\mathcal{H}_0+\mathcal{V}_0).\end{aligned} \tag{19d}$$

For simplicity, we will consider the dc-biased tight-binding model with time-harmonically varying impurity at site zero. In this case, Hamiltonian can be written in the localized Wannier basis as[10]

$$\mathcal{H}=\mathcal{H}_{\mathrm{TB}}+(V_0+V_1\cos\omega t)\left|0\right\rangle\left\langle 0\right|, \tag{20}$$

where V_0 characterizes the on-site energy of impurity and V_1 is the amplitude of an external harmonically driving electric field, which is assumed to reside at the impurity site ($n=0$ site).

Due to the special structure of Eq.(20), the definition of $g^{\mathrm{D}}(E)$ in Eq.(18) can be rewritten in the following form:

$$\begin{aligned}g^{\mathrm{D}}(E)&=\frac{1}{E-\mathcal{H}_{TB}-(\mathcal{V}_0+\mathcal{V}_{\mathrm{eff}})}\\&\equiv\frac{1}{E-\mathcal{H}_{TB}-[V_0+V_{\mathrm{eff}}(E)]\left|0\right\rangle\left\langle 0\right|}.\end{aligned} \tag{21}$$

By defining the free Green's function g^0:

$$g^0(E) = \frac{1}{E - \mathcal{H}_{\rm TB}}, \tag{22}$$

one can factorize $g^{\rm D}(E)$ in terms of Dyson's equation as follows:

$$g^{\rm D} = g^0 + g^0\left([V_0 + V_{\rm eff}(E)]|0\rangle\langle 0|\right) g^{\rm D}. \tag{23}$$

Iterating the above operator equation successively, and inserting the resulting operator equation into the localized Wannier basis: bra $\langle 0|$, and ket $|0\rangle$, the site-diagonal Floquet-Green's function can be deduced as follows:[14]

$$g^{\rm D}_{00}(E) = \frac{g^0_{00}}{1 - V(E) g^0_{00}}, \tag{24}$$

where $V(E) = V_0 + V_{\rm eff}(E)$.

Using the definition of $\mathcal{V}_{\rm eff}$ in Eqs.(17a)–(17d), one can express the $g^{\rm D}_{00}(E)$ in terms of the continued fraction as follows:

$$\begin{aligned}
g^{\rm D}_{00}(E) =& \frac{g^0_{00}}{1 - V(E) g^0_{00}} = \frac{1}{1/g^0_{00} - V(E)} \\
=& \left\{ \left(g_{00}^{0^{-1}}(E) - V_0\right) - \frac{1}{4}V_1^2 \left[\left(\left(g_{00}^{0^{-1}}(E+1) - V_0\right) - \cfrac{\frac{1}{4}V_1^2}{\left(g_{00}^{0^{-1}}(E+2) - V_0\right) - \cfrac{\frac{1}{4}V_1^2}{\vdots}} \right)^{-1} \right.\right. \\
& \left.\left. - \left(\left(g_{00}^{0^{-1}}(E-1) - V_0\right) - \cfrac{\frac{1}{4}V_1^2}{\left(g_{00}^{0^{-1}}(E-2) - V_0\right) - \cfrac{\frac{1}{4}V_1^2}{\vdots}} \right)^{-1} \right] \right\}^{-1} \\
=& \frac{2}{V_1} \left\{ \left(g_{00}^{0^{-1}}(E) - V_0\right) - \cfrac{\frac{V_1}{2}}{\frac{2}{V_1}\left(g_{00}^{0^{-1}}(E+1) - V_0\right) - \cfrac{1}{\vdots}} \right. \\
& \left. - \cfrac{\frac{V_1}{2}}{\frac{2}{V_1}\left(g_{00}^{0^{-1}}(E-1) - V_0\right) - \cfrac{1}{\vdots}} \right\}.
\end{aligned} \tag{25}$$

By comparing Eq.(20) with Eq.(6), it can be easily identified that $g_{00}^{0^{-1}}(E)$ is identical to $G_{00}^{-1}(E)$ defined in Eq.(11).

$$g_{00}^{0^{-1}}(E) = \left(\frac{\alpha}{\pi} \frac{\sin\left(\frac{E}{\alpha}\pi\right)}{J_{\frac{E}{\alpha}}\left(\frac{2t}{\alpha}\right) J_{-\frac{E}{\alpha}}\left(\frac{2t}{\alpha}\right)} \right). \tag{26}$$

The local density of states at the impurity site can be calculated from the diagonal elements of the Floquet–Green's function Eq.(25) through the formula,

$$\rho_0(E) = \mp\frac{1}{\pi}{\rm Im}\left(g^{\rm D}_{00}(E \pm {\rm i}\gamma)\right), \tag{27}$$

where γ is a positive infinitesimal quantity.

4. Numerical result and discussions

In order to give a clear picture of how the choice of parameters can influence the local density of states obtained in the previous section, we give a detailed numerical analysis. We firstly study the case where no impurity at site-0 is involved, we use the dimensionless parameters: hopping term t being set to be unity, and $V_0 = 0$. We gradually increase the parameter α, which characterizes the strength of the dc-biased field. The plots of local density of states are given in Figs.1(a)–1(d), where parameter α/t takes the values

of 0.01, 0.1, 1.0 and 2.0 respectively. In our numerical calculations, $\gamma = 10^{-8}$ unless otherwise specified. From the figures it can be seen that the profiles of local density of states resemble those of tight-binding Hamiltonian in the absence of driving dc fields, when α/t is small. In this case, weak electric field strength just slightly modifies the contour of local density of states, so almost no localized state appears in the weak driving electric fields. When the strength of electric field α increases up to the value comparable with the hopping parameter t, discrete spectrum can be identified in the local density of states, which demonstrates the appearance of the resonant localized states. With the introduction of the external dc electric fields, the degeneracy among electronic states from different potential wells of periodic solids is lifted,[19,20] leading to the localized electronic states.

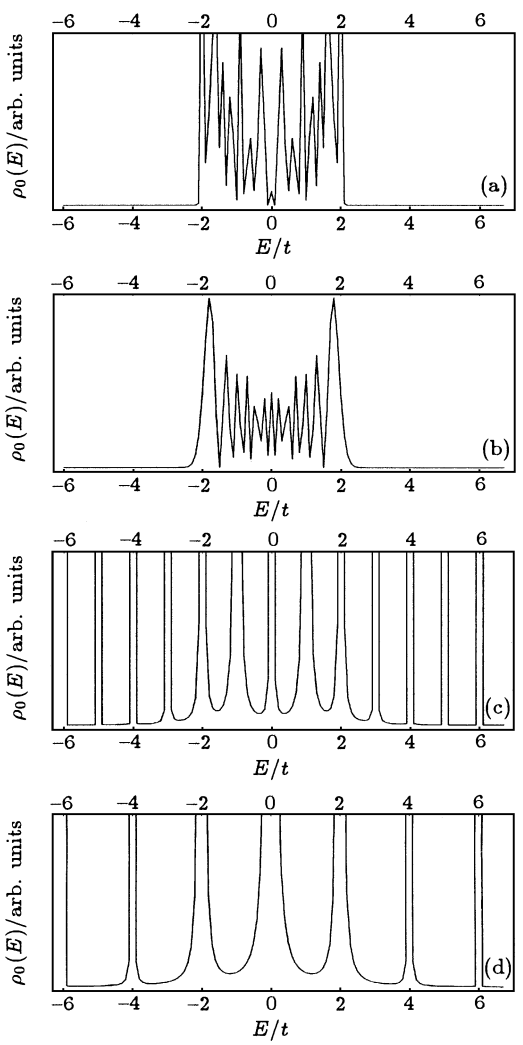


Fig.1. The local density of states in a perfect dc-biased superlattices.

What will happen if the time-harmonically varying impurity dwelling on the site zero is introduced? We show the influence of impurity on the local density of states in Figs.2(a)–(c), where $V_1/\hbar\omega$ takes the values 0.20, 2.00, and 3.00 respectively from top to bottom. The other parameters used in this figure are the same as those in Fig.1 except that $\alpha/\hbar\omega = t/\hbar\omega$ is set to be unity. From Figs.2(a)–(c), it can be clearly seen that the introduction of the harmonically driving impurity almost leaves the local density of states unaltered when $V_1/\hbar\omega$ is tiny; while the increase in the ratio $V_1/\hbar\omega$ leads to the generation of the new states between the neighbouring Wannier–Stark localized gaps. That is to say, the new localized states will appear due to the harmonically driving impurity. This phenomenon will become more prominent, when the strength of the harmonically driving field becomes stronger.

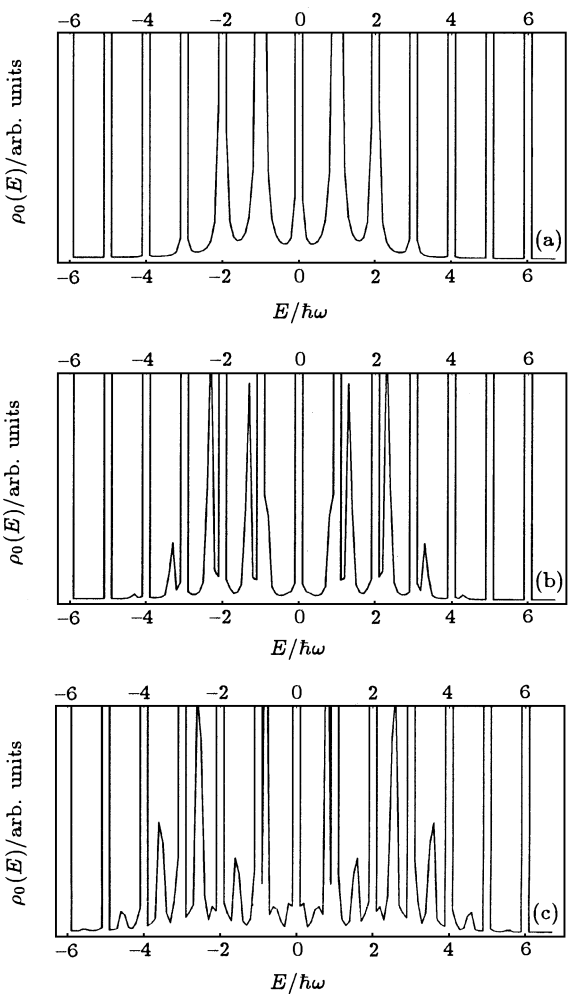


Fig.2. The local density of states in a dc-biased superlattices with a harmonically driving field at site zero.

In summary, by using the Floquet–Green's formalism, we have obtained the analytical continued fraction expression of local density of states of a dc-biased tight-binding model with single-site impurity

potential varying harmonically with time. The numerical analysis shows that the larger value of the strength of the harmonically driving field will lead to more new states emerging between the neighbouring resonant Wannier–Stark localized states. It is noticeable that the local density of states is closely related to the tunnelling currents in various hybrid nanostructures, the results presented here may provide a qualitative way to alter the tunnelling current through the introduction of time-dependent impurity.

References

[1] Feldmann J, Leo K, Shah J, Miller D A B and Cunningham J E 1992 *Phys. Rev.* B **46** 7252

[2] Leo K, Haring Bolivar P, Brügemann F, Schwedler R and Köhler K 1992 *Solid State Commun.* **84** 943

[3] Waschke C, Roskos H G, Schwedler R, Leo K and Kurz H 1993 *Phys. Rev. Lett.* **70** 3319

[4] Tsu R and Dohler G H 1975 *Phys. Rev.* B **12** 680

[5] Dignam M M and de Sterke C M 2002 *Phys. Rev. Lett.* **88** 046806

[6] Zhao X G, Jahnke R and Niu Q 1995 *Phys. Lett.* A **202** 297

[7] Holthaus M 1992 *Phys. Rev. Lett.* **69** 351

[8] Löser F, Dignam M M, Kosevich Yu A Köhler K and Leo K 2000 *Phys. Rev. Lett.* **85** 4763

[9] Duan S Q, Wang Z G, Wu B Y and Zhao X G 2004 *Phys. Lett.* A **320** 63

[10] Zhang A Z, Zhang P, Duan S Q, Zhao X G and Liang J Q 2001 *Chin. Phys.* **10** 537

[11] Johnsen K and Jauho AP 1999 *Phys. Rev. Lett.* **83** 1207

[12] Guo R M, Shi H Y and Sun X D 2004 *Acta Phys. Sin.* **53** 3487 (in Chinese)

[13] Nordstrom K B, Johnsen K Allen S J, Jauho A P, Birnir B, Kono J, Noda T, Akiyama H and Sakaki H 1998 *Phys. Rev. Lett.* **81** 457

[14] Martinez D F 2003 *J. Phys. A: Math. Gen.* **36** 9827

[15] Peskin U and Moiseyev N 1993 *J. Chem. Phys.* **99** 4590

[16] Grosso G and Parravicini G 2000 *Solid State Physics* (San Diego: Academic Press)

[17] Economou E N 1990 *Green's Function in Quantum physics* (2nd Ed.) (Berlin: Springer)

[18] Aulbur W G, Jönsson L and Wilkins J W 2000 *Solid State Phys.* **54** 1

[19] Emin D and Hart C F 1987 *Phys. Rev.* B **36** 7353

[20] Wang H M and Zhang Y F 2005 *Acta Phys. Sin.* **54** 2226